



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:37 AM GMT

PDB ID : 3FAA  
Title : Crystal structure of TGFbRI complexed with a 2-aminoimidazole inhibitor  
Authors : Boriack-Sjodin, P.A.; Fitch, C.  
Deposited on : 2008-11-16  
Resolution : 3.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

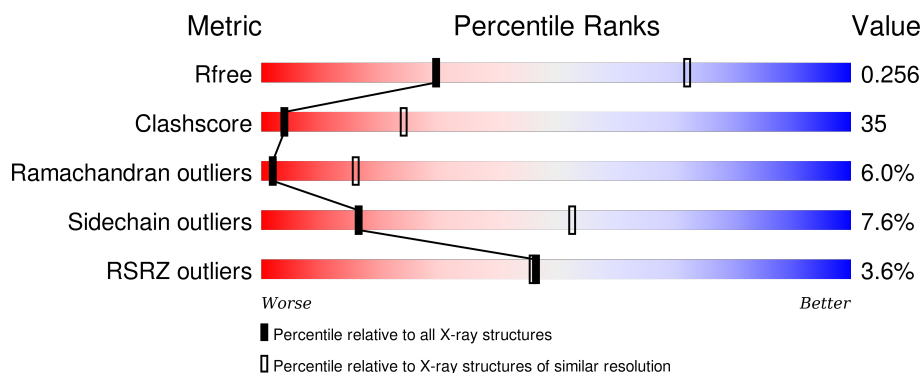
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1005 (3.42-3.30)
Clashscore	102246	1076 (3.42-3.30)
Ramachandran outliers	100387	1059 (3.42-3.30)
Sidechain outliers	100360	1058 (3.42-3.30)
RSRZ outliers	91569	1010 (3.42-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	342	<div> <div>3%</div> <div>44%</div> <div>45%</div> <div>7%</div> <div>.</div> </div>
1	B	342	<div> <div>50%</div> <div>36%</div> <div>8%</div> <div>5%</div> </div>
1	C	342	<div> <div>12%</div> <div>32%</div> <div>56%</div> <div>8%</div> <div>.</div> </div>
1	D	342	<div> <div>%</div> <div>45%</div> <div>45%</div> <div>6%</div> <div>.</div> </div>
1	E	342	<div> <div>%</div> <div>46%</div> <div>43%</div> <div>7%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	A	9	-	-	X	-
3	PO4	B	12	-	-	-	X
3	PO4	D	13	-	-	X	-
3	PO4	D	14	-	-	-	X
3	PO4	D	24	-	-	-	X
3	PO4	E	2	-	-	X	-

## 2 Entry composition [i](#)

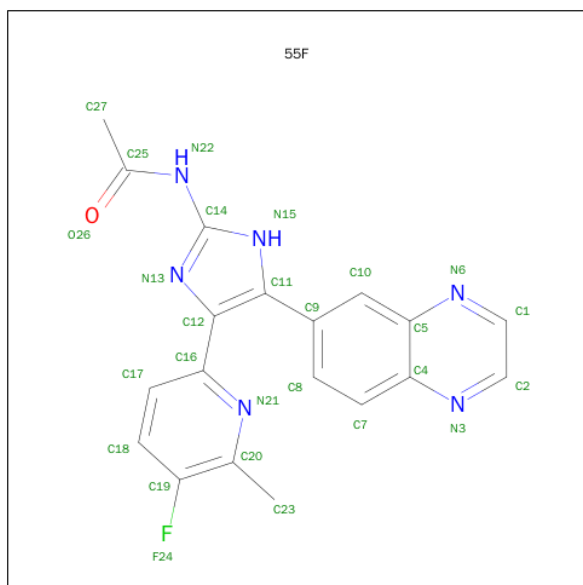
There are 3 unique types of molecules in this entry. The entry contains 13294 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called TGF-beta receptor type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	0	0
			2617	1650	469	482	16			
1	B	324	Total	C	N	O	S	0	0	0
			2590	1636	463	475	16			
1	C	330	Total	C	N	O	S	0	0	0
			2629	1658	471	484	16			
1	D	330	Total	C	N	O	S	0	0	0
			2629	1658	471	484	16			
1	E	330	Total	C	N	O	S	0	0	0
			2629	1658	471	484	16			

- Molecule 2 is N-[4-(5-FLUORO-6-METHYLPYRIDIN-2-YL)-5-QUINOXALIN-6-YL-1H-IMIDAZOL-2-YL]ACETAMIDE (three-letter code: 55F) (formula: C<sub>19</sub>H<sub>15</sub>FN<sub>6</sub>O).



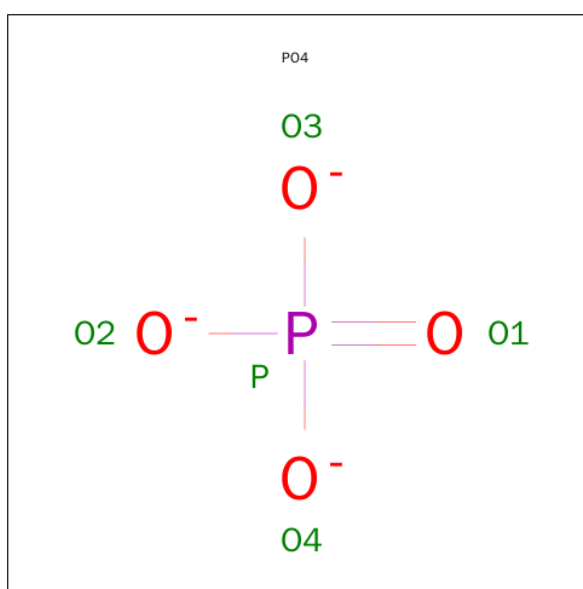
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			27	19	1	6	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	F	N	O	0	0
			27	19	1	6	1		
2	C	1	Total	C	F	N	O	0	0
			27	19	1	6	1		
2	D	1	Total	C	F	N	O	0	0
			27	19	1	6	1		
2	E	1	Total	C	F	N	O	0	0
			27	19	1	6	1		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total	O P	0	0
			5	4 1		
3	E	1	Total	O P	0	0
			5	4 1		
3	B	1	Total	O P	0	0
			5	4 1		
3	A	1	Total	O P	0	0
			5	4 1		
3	C	1	Total	O P	0	0
			5	4 1		
3	B	1	Total	O P	0	0
			5	4 1		
3	D	1	Total	O P	0	0
			5	4 1		

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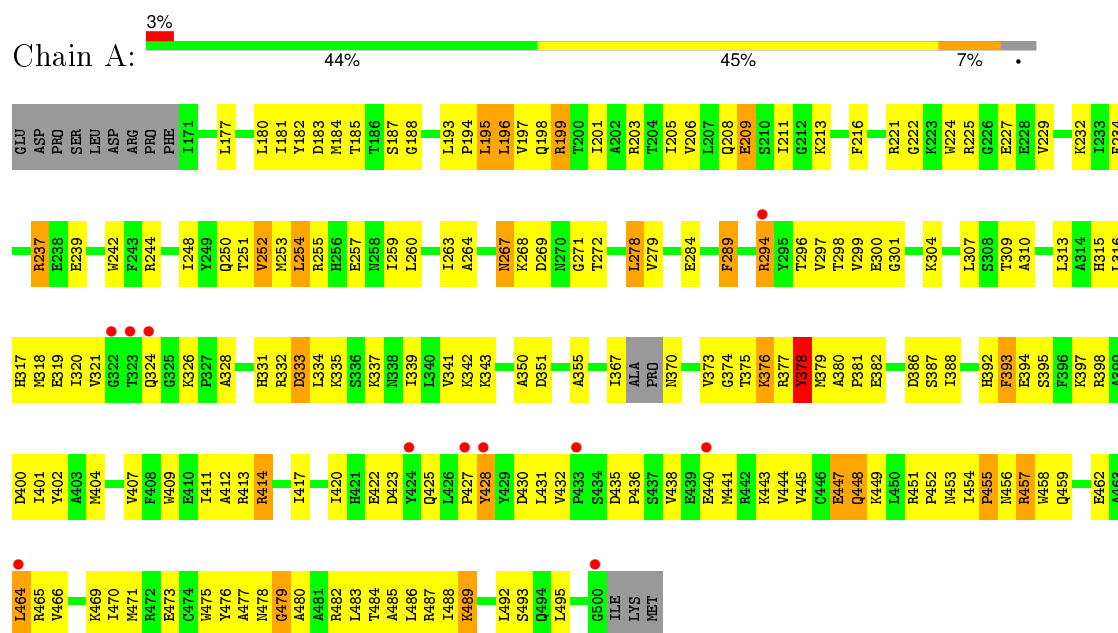
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		

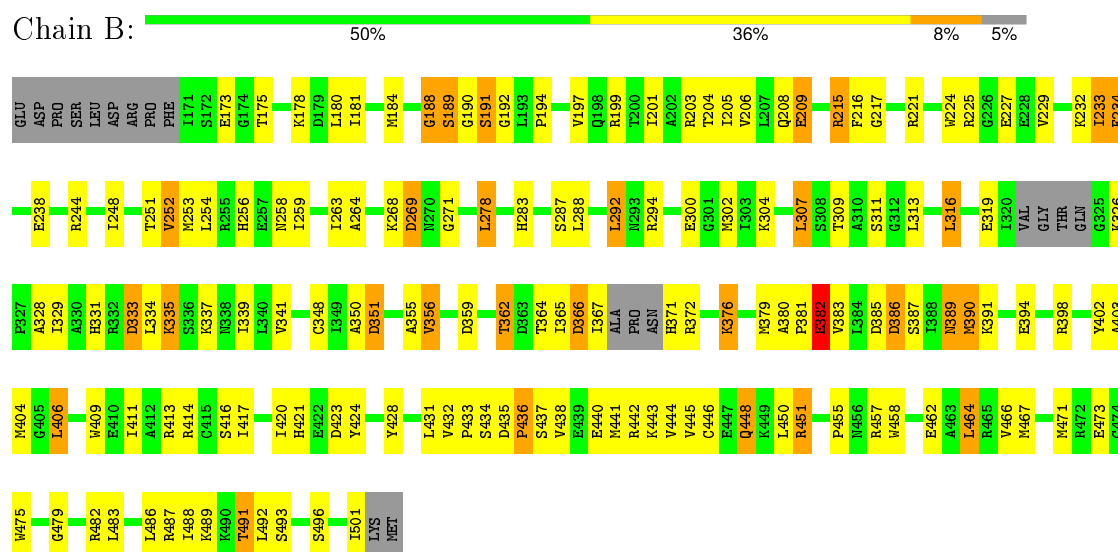
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

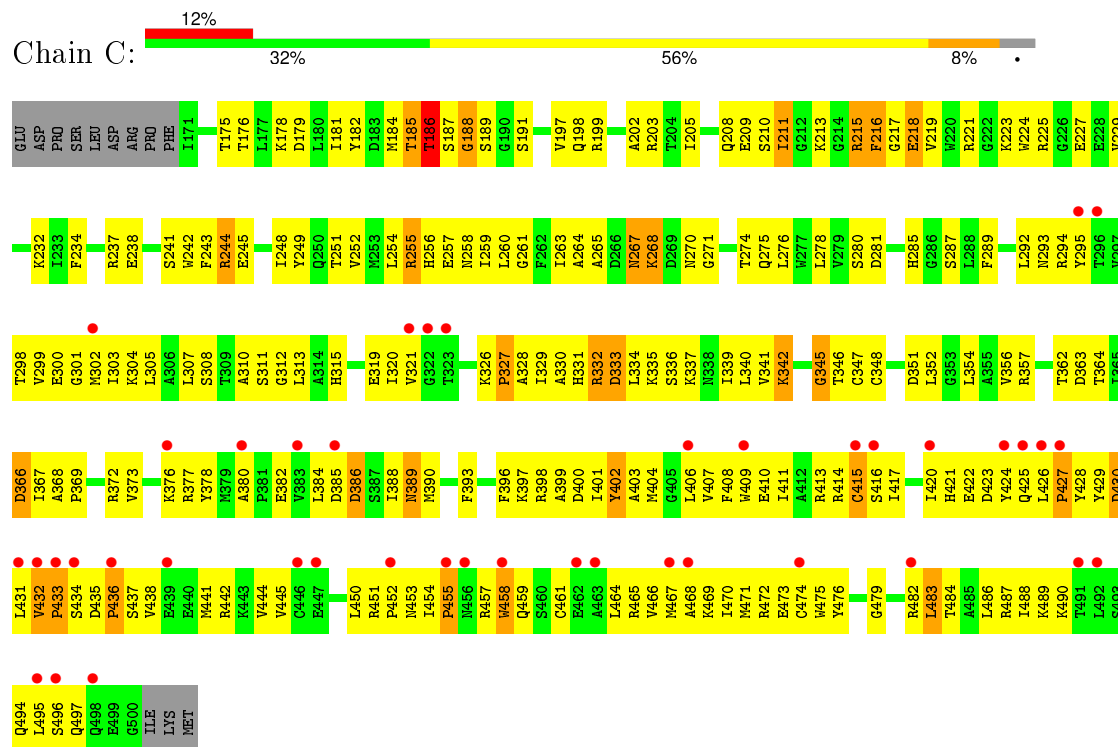
#### • Molecule 1: TGF-beta receptor type-1



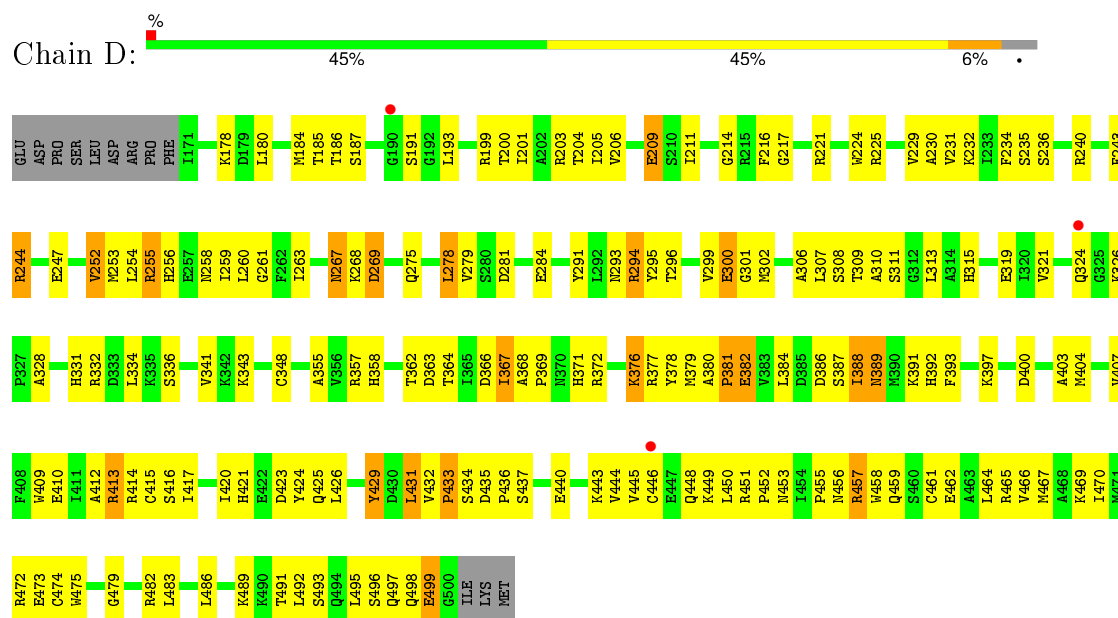
#### • Molecule 1: TGF-beta receptor type-1



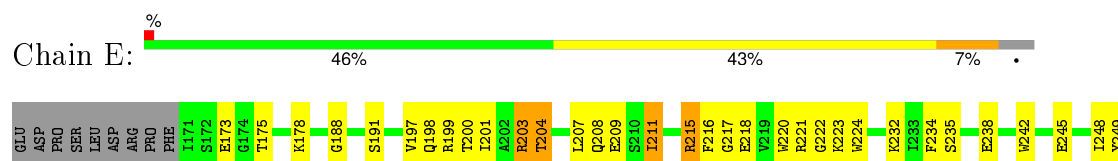
• Molecule 1: TGF-beta receptor type-1



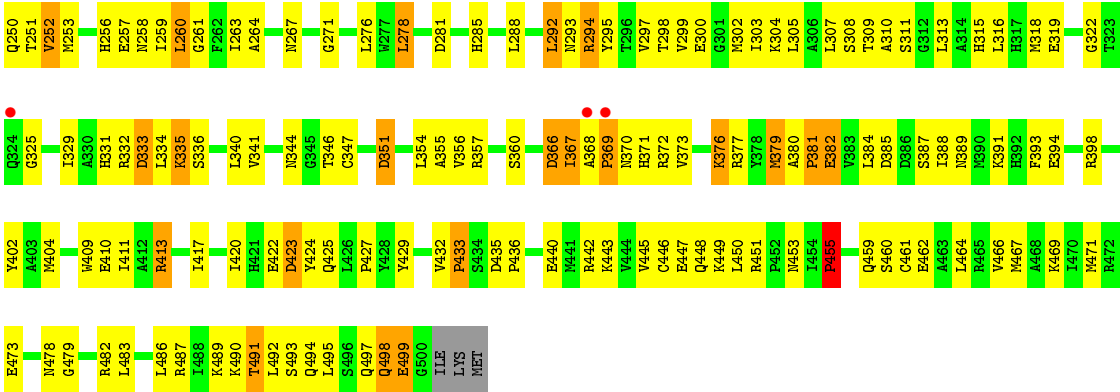
• Molecule 1: TGF-beta receptor type-1



• Molecule 1: TGF-beta receptor type-1







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	174.86Å 248.85Å 138.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 3.35 47.69 – 3.19	Depositor EDS
% Data completeness (in resolution range)	99.8 (35.00-3.35) 98.4 (47.69-3.19)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.09 (at 3.19Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.228 , 0.271 0.212 , 0.256	Depositor DCC
$R_{free}$ test set	2200 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	82.5	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 71.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 49780 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13294	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, 55F

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.36	0/2668	0.62	1/3600 (0.0%)
1	B	0.46	0/2640	0.66	0/3560
1	C	0.37	0/2682	0.64	0/3622
1	D	0.44	0/2682	0.67	0/3622
1	E	0.48	0/2682	0.70	0/3622
All	All	0.42	0/13354	0.66	1/18026 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	268	LYS	N-CA-C	5.35	125.44	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2617	0	2618	189	0
1	B	2590	0	2595	150	0
1	C	2629	0	2631	259	0
1	D	2629	0	2631	165	0
1	E	2629	0	2631	167	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	27	0	15	1	0
2	B	27	0	15	2	0
2	C	27	0	15	1	0
2	D	27	0	15	0	0
2	E	27	0	15	2	0
3	A	15	0	0	2	0
3	B	15	0	0	1	0
3	C	5	0	0	0	0
3	D	15	0	0	2	0
3	E	15	0	0	2	0
All	All	13294	0	13181	919	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 35.

All (919) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:417:ILE:HD11	1:D:457:ARG:HH12	1.08	1.11
1:E:367:ILE:HD13	1:E:370:ASN:HD21	1.21	1.02
1:D:367:ILE:HG13	1:D:369:PRO:HD3	1.39	1.02
1:A:417:ILE:HD11	1:A:457:ARG:HH12	1.26	0.99
1:E:256:HIS:HD2	1:E:258:ASN:H	0.99	0.98
1:C:298:THR:HG22	1:C:300:GLU:H	1.28	0.97
1:A:376:LYS:HE3	1:A:438:VAL:HG13	1.49	0.94
1:D:253:MET:HB2	1:D:326:LYS:HB2	1.50	0.94
1:E:487:ARG:HH21	1:E:490:LYS:HD2	1.35	0.92
1:C:216:PHE:HD1	1:C:217:GLY:N	1.67	0.91
1:B:406:LEU:HD12	1:B:406:LEU:H	1.34	0.90
1:D:368:ALA:HB2	1:E:178:LYS:HE3	1.52	0.90
1:C:267:ASN:HD22	1:C:267:ASN:H	1.14	0.89
1:A:298:THR:HG22	1:A:300:GLU:H	1.38	0.89
1:B:389:ASN:HD21	1:B:391:LYS:HD3	1.37	0.88
1:E:367:ILE:CD1	1:E:370:ASN:HD21	1.88	0.85
1:A:267:ASN:H	1:A:267:ASN:HD22	1.20	0.84
1:A:309:THR:HG22	1:A:404:MET:HE2	1.60	0.84
1:E:256:HIS:CD2	1:E:258:ASN:H	1.90	0.84
1:B:443:LYS:HG2	1:B:448:GLN:HE21	1.43	0.83
1:C:216:PHE:CD1	1:C:217:GLY:N	2.46	0.83
1:B:403:ALA:HA	1:B:406:LEU:HD13	1.58	0.83
1:C:417:ILE:HD13	1:C:461:CYS:SG	2.19	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:436:PRO:HB3	1:C:441:MET:SD	2.18	0.83
1:D:417:ILE:HD11	1:D:457:ARG:NH1	1.93	0.82
1:B:252:VAL:HG23	1:B:253:MET:H	1.44	0.82
1:E:256:HIS:HD2	1:E:258:ASN:N	1.78	0.81
1:C:267:ASN:ND2	1:C:267:ASN:H	1.78	0.81
1:A:388:ILE:HD11	1:A:395:SER:HB3	1.62	0.81
1:B:311:SER:HA	1:B:489:LYS:HG3	1.63	0.81
1:E:367:ILE:HD13	1:E:370:ASN:ND2	1.95	0.80
1:C:409:TRP:HB2	1:C:471:MET:HE1	1.62	0.80
1:C:461:CYS:HB2	1:C:464:LEU:HD23	1.62	0.80
1:B:252:VAL:HG21	1:B:326:LYS:HA	1.63	0.79
1:C:368:ALA:N	1:C:369:PRO:HD2	1.98	0.79
1:A:443:LYS:HE2	1:A:448:GLN:NE2	1.98	0.79
1:C:335:LYS:CG	1:C:336:SER:H	1.96	0.79
1:B:199:ARG:HD2	1:B:203:ARG:NH1	1.98	0.79
1:A:216:PHE:HE2	1:A:232:LYS:HG3	1.48	0.79
1:A:413:ARG:HH11	1:A:413:ARG:HG2	1.47	0.79
1:D:252:VAL:HG23	1:D:253:MET:H	1.47	0.78
1:C:417:ILE:O	1:C:420:ILE:HG12	1.84	0.78
1:C:202:ALA:HA	1:C:205:ILE:HD12	1.65	0.77
1:A:470:ILE:HA	1:A:473:GLU:HB2	1.65	0.76
1:D:457:ARG:HB2	1:D:457:ARG:NH1	1.99	0.76
1:A:417:ILE:HD11	1:A:457:ARG:NH1	2.01	0.76
1:C:372:ARG:NH2	1:C:438:VAL:HG21	2.01	0.76
1:A:267:ASN:N	1:A:267:ASN:HD22	1.80	0.75
1:C:367:ILE:HG23	1:C:369:PRO:HG2	1.65	0.75
1:A:224:TRP:CH2	1:A:225:ARG:HD2	2.20	0.75
1:C:332:ARG:HB3	1:C:332:ARG:NH1	2.02	0.74
1:B:309:THR:HG22	1:B:404:MET:CE	2.17	0.74
1:A:469:LYS:HE2	1:A:473:GLU:HG3	1.69	0.74
1:C:256:HIS:HB3	1:C:259:ILE:HG13	1.69	0.74
1:E:368:ALA:HB3	1:E:369:PRO:HD3	1.68	0.74
1:C:444:VAL:HG13	1:C:450:LEU:HD12	1.70	0.74
1:D:433:PRO:HG2	1:D:440:GLU:OE2	1.87	0.74
1:C:487:ARG:NH2	1:C:490:LYS:HD2	2.02	0.74
1:E:377:ARG:HH12	3:E:2:PO4:P	2.11	0.73
1:A:428:TYR:HE2	1:A:445:VAL:HG22	1.53	0.73
1:C:302:MET:HG3	1:C:411:ILE:HG22	1.69	0.73
1:A:453:ASN:O	1:A:455:PRO:HD3	1.89	0.73
1:C:454:ILE:HD11	1:C:475:TRP:CZ3	2.23	0.73
1:C:215:ARG:N	1:C:215:ARG:HE	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:435:ASP:N	1:C:436:PRO:HD3	2.03	0.73
1:C:410:GLU:HB3	1:C:424:TYR:HE1	1.52	0.73
1:B:376:LYS:H	1:B:376:LYS:HD2	1.54	0.72
1:C:414:ARG:HD3	1:C:424:TYR:N	2.04	0.72
1:D:372:ARG:HD3	1:D:379:MET:SD	2.30	0.72
1:A:466:VAL:HG21	1:A:495:LEU:HD22	1.72	0.72
1:C:299:VAL:HG22	1:C:415:CYS:SG	2.30	0.71
1:A:319:GLU:HB2	1:A:328:ALA:HB2	1.72	0.71
1:C:479:GLY:HA2	1:C:482:ARG:HD2	1.72	0.71
1:E:487:ARG:O	1:E:491:THR:HG23	1.90	0.71
1:A:289:PHE:CD2	1:A:337:LYS:HE2	2.24	0.71
1:B:233:ILE:HD13	1:B:233:ILE:O	1.90	0.71
1:E:487:ARG:HH21	1:E:490:LYS:CD	2.02	0.71
1:B:201:ILE:O	1:B:205:ILE:HG13	1.90	0.71
1:C:307:LEU:HD23	1:C:307:LEU:O	1.90	0.71
1:D:462:GLU:O	1:D:466:VAL:HG23	1.90	0.71
1:C:181:ILE:O	1:C:185:THR:HG22	1.91	0.70
1:C:335:LYS:HG3	1:C:336:SER:H	1.55	0.70
1:A:380:ALA:HA	1:A:402:TYR:CE1	2.27	0.70
1:C:335:LYS:CG	1:C:336:SER:N	2.54	0.70
1:E:303:ILE:HD13	1:E:495:LEU:HG	1.73	0.70
1:A:466:VAL:O	1:A:470:ILE:HG13	1.92	0.70
1:E:313:LEU:HD13	1:E:334:LEU:HD11	1.74	0.70
1:C:384:LEU:HD22	1:C:442:ARG:HB2	1.73	0.70
1:D:307:LEU:HA	1:D:492:LEU:HD23	1.74	0.69
1:A:459:GLN:OE1	1:A:465:ARG:HG2	1.92	0.69
1:D:497:GLN:HG2	1:D:497:GLN:O	1.91	0.69
1:C:332:ARG:HB3	1:C:332:ARG:HH11	1.57	0.69
1:D:310:ALA:HA	1:D:404:MET:HE1	1.74	0.69
1:C:459:GLN:HE22	1:C:465:ARG:HG3	1.56	0.69
1:B:406:LEU:HD12	1:B:406:LEU:N	2.08	0.69
1:E:459:GLN:NE2	1:E:459:GLN:HA	2.05	0.69
1:E:459:GLN:HE21	1:E:459:GLN:HA	1.58	0.69
1:C:256:HIS:HB3	1:C:259:ILE:CD1	2.22	0.69
1:D:315:HIS:O	1:D:326:LYS:HE3	1.92	0.69
1:D:431:LEU:HD22	1:D:444:VAL:HG13	1.75	0.69
1:C:413:ARG:HD3	1:C:423:ASP:O	1.94	0.68
1:B:406:LEU:H	1:B:406:LEU:CD1	2.06	0.68
1:E:332:ARG:HH22	1:E:369:PRO:HG2	1.58	0.68
1:C:469:LYS:O	1:C:473:GLU:HG3	1.93	0.68
1:B:450:LEU:O	1:B:451:ARG:HD3	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:298:THR:HG22	1:E:299:VAL:N	2.10	0.67
1:C:398:ARG:HB3	1:C:482:ARG:HH11	1.59	0.67
1:C:267:ASN:N	1:C:267:ASN:ND2	2.37	0.67
1:C:483:LEU:HD13	1:C:488:ILE:HD11	1.77	0.67
1:A:313:LEU:HD11	1:A:317:HIS:HE2	1.58	0.67
1:D:357:ARG:HB2	1:D:366:ASP:HB2	1.76	0.67
1:C:258:ASN:O	1:C:348:CYS:HA	1.94	0.67
1:E:490:LYS:O	1:E:493:SER:HB2	1.94	0.67
1:B:493:SER:O	1:B:496:SER:HB3	1.95	0.67
1:D:417:ILE:HG13	1:D:420:ILE:HG13	1.77	0.67
1:E:204:THR:HG22	1:E:224:TRP:NE1	2.09	0.67
1:B:178:LYS:HD2	1:B:227:GLU:OE2	1.95	0.67
1:D:469:LYS:O	1:D:473:GLU:HG2	1.95	0.66
1:B:309:THR:HG22	1:B:404:MET:HE2	1.77	0.66
1:A:317:HIS:HB3	1:A:397:LYS:HE2	1.76	0.66
1:C:285:HIS:HD2	1:C:342:LYS:O	1.79	0.66
1:B:409:TRP:HA	1:B:471:MET:HE1	1.76	0.66
1:C:372:ARG:HH12	1:C:438:VAL:HG11	1.61	0.66
1:C:232:LYS:HD2	1:C:234:PHE:CZ	2.30	0.66
1:C:420:ILE:HG13	1:C:420:ILE:O	1.94	0.66
1:A:469:LYS:HE2	1:A:473:GLU:CG	2.26	0.66
1:C:256:HIS:HB3	1:C:259:ILE:CG1	2.26	0.66
1:D:184:MET:CE	1:D:193:LEU:HG	2.26	0.66
1:E:334:LEU:O	1:E:335:LYS:HB3	1.96	0.65
1:D:216:PHE:CD1	1:D:217:GLY:N	2.64	0.65
1:E:298:THR:HG22	1:E:300:GLU:H	1.61	0.65
1:A:267:ASN:ND2	1:A:267:ASN:N	2.41	0.65
1:C:268:LYS:HB2	1:C:275:GLN:HB2	1.78	0.65
1:D:263:ILE:HB	1:D:279:VAL:HG12	1.78	0.65
1:A:309:THR:HG22	1:A:404:MET:CE	2.25	0.65
1:B:376:LYS:HA	1:B:379:MET:CE	2.25	0.65
1:E:198:GLN:HE22	1:E:250:GLN:HE22	1.45	0.65
1:A:409:TRP:HD1	1:A:471:MET:HE1	1.62	0.64
1:D:199:ARG:HD2	1:D:203:ARG:CZ	2.28	0.64
1:E:331:HIS:O	1:E:332:ARG:HB2	1.97	0.64
1:B:248:ILE:CD1	1:B:355:ALA:HB3	2.28	0.64
1:D:294:ARG:HD3	1:D:295:TYR:CE2	2.31	0.64
1:E:245:GLU:HG2	1:E:249:TYR:HE1	1.63	0.64
1:C:453:ASN:O	1:C:455:PRO:HD3	1.97	0.64
1:D:466:VAL:O	1:D:469:LYS:HB3	1.98	0.64
1:C:334:LEU:HD23	1:C:335:LYS:N	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:LEU:HD11	1:C:259:ILE:HG21	1.80	0.63
1:C:474:CYS:SG	1:C:483:LEU:HD11	2.38	0.63
1:D:209:GLU:OE2	1:D:221:ARG:NH1	2.29	0.63
1:C:320:ILE:HG22	1:C:321:VAL:N	2.13	0.63
1:D:254:LEU:HD11	1:D:259:ILE:HG21	1.80	0.63
1:D:457:ARG:CB	1:D:457:ARG:HH11	2.12	0.63
1:C:334:LEU:HD23	1:C:335:LYS:H	1.62	0.63
1:C:473:GLU:HA	1:C:476:TYR:CZ	2.32	0.63
1:C:473:GLU:HB3	1:C:483:LEU:HG	1.80	0.63
1:C:413:ARG:HG3	1:C:422:GLU:HB2	1.81	0.63
1:B:381:PRO:HD2	1:B:482:ARG:HH22	1.63	0.63
1:B:376:LYS:HA	1:B:379:MET:HE3	1.80	0.63
1:D:451:ARG:HG2	1:D:475:TRP:HB3	1.80	0.63
1:A:486:LEU:O	1:A:489:LYS:HB3	1.99	0.63
1:D:178:LYS:HD2	1:D:178:LYS:N	2.13	0.63
1:C:410:GLU:HB3	1:C:424:TYR:CE1	2.33	0.63
1:E:409:TRP:HA	1:E:471:MET:HE1	1.79	0.63
1:B:414:ARG:HD2	1:B:424:TYR:HB2	1.81	0.62
1:D:229:VAL:HG11	1:D:279:VAL:HG13	1.81	0.62
1:A:428:TYR:CE2	1:A:445:VAL:HG22	2.35	0.62
1:A:208:GLN:HG2	1:A:222:GLY:HA2	1.79	0.62
1:A:248:ILE:HA	1:A:251:THR:HG23	1.82	0.62
1:E:367:ILE:CG1	1:E:370:ASN:HD21	2.12	0.62
1:C:377:ARG:HE	1:C:436:PRO:HG2	1.64	0.62
1:E:318:MET:HG2	1:E:319:GLU:N	2.15	0.62
1:D:457:ARG:CB	1:D:457:ARG:NH1	2.62	0.62
1:C:384:LEU:HD13	1:C:442:ARG:HA	1.79	0.62
1:A:267:ASN:ND2	1:A:267:ASN:H	1.95	0.62
1:A:398:ARG:CZ	1:A:480:ALA:HA	2.30	0.62
1:C:305:LEU:HD13	1:C:305:LEU:O	1.99	0.62
1:A:378:TYR:HD1	1:A:378:TYR:H	1.46	0.62
1:C:398:ARG:HD3	1:C:479:GLY:HA3	1.82	0.62
1:E:253:MET:HE3	1:E:325:GLY:HA2	1.81	0.62
1:C:303:ILE:O	1:C:307:LEU:HB2	2.00	0.61
1:D:216:PHE:CG	1:D:217:GLY:N	2.68	0.61
1:A:199:ARG:HD2	1:A:203:ARG:CZ	2.30	0.61
1:E:389:ASN:HD21	1:E:391:LYS:HB3	1.65	0.61
1:B:479:GLY:HA2	1:B:482:ARG:HD2	1.82	0.61
1:D:368:ALA:HB2	1:E:178:LYS:CE	2.29	0.61
1:B:334:LEU:O	1:B:335:LYS:HB3	1.99	0.61
1:B:319:GLU:HB2	1:B:328:ALA:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:ALA:HA	1:A:402:TYR:CD1	2.36	0.61
1:D:431:LEU:HD11	1:D:450:LEU:HD13	1.81	0.61
1:B:316:LEU:HD22	1:B:329:ILE:HB	1.82	0.61
1:B:199:ARG:HD2	1:B:203:ARG:CZ	2.31	0.61
1:A:248:ILE:O	1:A:251:THR:HG23	2.00	0.61
1:E:433:PRO:HG2	1:E:440:GLU:OE2	2.01	0.61
1:A:294:ARG:O	1:A:294:ARG:HD3	2.01	0.61
1:D:243:PHE:CZ	1:E:175:THR:HG23	2.35	0.61
1:D:252:VAL:HG23	1:D:253:MET:N	2.16	0.61
1:C:461:CYS:CB	1:C:464:LEU:HD23	2.29	0.61
1:C:258:ASN:OD1	1:C:308:SER:HB2	2.01	0.61
1:D:437:SER:OG	1:D:440:GLU:HG3	2.01	0.61
1:A:367:ILE:HD12	1:A:370:ASN:HB2	1.83	0.61
1:D:296:THR:HG21	1:D:421:HIS:CD2	2.35	0.61
1:C:495:LEU:HG	1:C:495:LEU:O	2.01	0.61
1:C:384:LEU:HD23	1:C:438:VAL:HG13	1.81	0.60
1:E:200:THR:O	1:E:204:THR:HB	2.01	0.60
1:D:413:ARG:O	1:D:414:ARG:HG2	2.01	0.60
1:A:211:ILE:HD12	1:A:211:ILE:O	2.01	0.60
1:C:377:ARG:CG	1:C:436:PRO:HG2	2.31	0.60
1:C:414:ARG:HD3	1:C:424:TYR:H	1.65	0.60
1:C:217:GLY:O	1:C:218:GLU:HB2	2.02	0.60
1:C:397:LYS:O	1:C:401:ILE:HG12	2.01	0.60
1:C:479:GLY:HA2	1:C:482:ARG:CD	2.32	0.60
1:D:498:GLN:O	1:D:499:GLU:HG3	2.01	0.60
1:D:343:LYS:HB2	3:D:13:PO4:O4	2.02	0.60
1:C:466:VAL:O	1:C:470:ILE:HG13	2.01	0.60
1:B:302:MET:HE1	1:B:467:MET:HG3	1.84	0.60
1:C:434:SER:C	1:C:436:PRO:HD3	2.22	0.60
1:B:252:VAL:HG23	1:B:253:MET:N	2.16	0.60
1:E:356:VAL:HG23	1:E:393:PHE:HE1	1.66	0.60
1:B:309:THR:HG22	1:B:404:MET:HE1	1.82	0.60
1:B:362:THR:O	1:B:364:THR:HG23	2.02	0.60
1:C:287:SER:HB2	1:C:337:LYS:HA	1.84	0.59
1:C:352:LEU:N	1:C:352:LEU:HD23	2.16	0.59
1:A:289:PHE:CE2	1:A:337:LYS:HE2	2.38	0.59
1:D:267:ASN:N	1:D:267:ASN:OD1	2.34	0.59
1:D:469:LYS:HD2	1:D:472:ARG:HH21	1.67	0.59
1:A:209:GLU:OE2	1:A:221:ARG:NH1	2.31	0.59
1:B:178:LYS:HG2	1:C:368:ALA:HB3	1.85	0.59
1:A:216:PHE:CE2	1:A:232:LYS:HG3	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:335:LYS:HG2	1:C:336:SER:N	2.17	0.59
1:C:372:ARG:NH1	1:C:438:VAL:HG11	2.16	0.59
1:B:376:LYS:N	1:B:376:LYS:HD2	2.18	0.59
1:C:409:TRP:CB	1:C:471:MET:HE1	2.30	0.59
1:E:204:THR:CG2	1:E:224:TRP:HE1	2.16	0.59
1:E:413:ARG:NH1	1:E:423:ASP:O	2.36	0.59
1:C:261:GLY:HA3	1:C:281:ASP:OD2	2.02	0.59
1:B:359:ASP:OD2	1:B:362:THR:HG23	2.03	0.58
1:D:205:ILE:CG2	1:D:206:VAL:N	2.65	0.58
1:E:447:GLU:O	1:E:449:LYS:HG3	2.04	0.58
1:B:251:THR:HG23	1:B:252:VAL:HG22	1.86	0.58
1:C:385:ASP:HA	1:C:442:ARG:CD	2.33	0.58
1:D:205:ILE:HG22	1:D:206:VAL:N	2.16	0.58
1:E:425:GLN:OE1	1:E:429:TYR:CD1	2.56	0.58
1:B:302:MET:CE	1:B:467:MET:HG3	2.33	0.58
1:C:357:ARG:HB2	1:C:366:ASP:HB2	1.85	0.58
1:E:332:ARG:NH2	1:E:369:PRO:HG2	2.18	0.58
1:A:476:TYR:C	1:A:478:ASN:H	2.07	0.58
1:D:389:ASN:ND2	1:D:391:LYS:H	2.02	0.58
1:A:431:LEU:HD13	1:A:444:VAL:HG11	1.86	0.58
1:E:469:LYS:HG3	1:E:473:GLU:OE2	2.03	0.58
1:B:365:ILE:HG13	1:B:367:ILE:HB	1.85	0.58
1:C:368:ALA:N	1:C:369:PRO:CD	2.66	0.58
1:D:378:TYR:OH	1:D:410:GLU:OE2	2.19	0.58
1:E:367:ILE:N	1:E:367:ILE:HD12	2.20	0.57
1:C:417:ILE:HD12	1:C:457:ARG:NH1	2.19	0.57
1:C:403:ALA:O	1:C:407:VAL:HG23	2.04	0.57
1:E:245:GLU:HG2	1:E:249:TYR:CE1	2.39	0.57
1:D:459:GLN:HE21	1:D:465:ARG:NH1	2.01	0.57
1:C:382:GLU:HB3	1:C:388:ILE:HB	1.86	0.57
1:A:470:ILE:CD1	1:A:492:LEU:HD11	2.33	0.57
1:D:431:LEU:HD11	1:D:450:LEU:HD22	1.86	0.57
1:D:293:ASN:ND2	1:D:424:TYR:CG	2.71	0.57
1:D:229:VAL:CG1	1:D:279:VAL:HG13	2.34	0.57
1:C:308:SER:OG	1:C:347:CYS:HB2	2.04	0.57
1:D:498:GLN:O	1:D:499:GLU:CG	2.52	0.57
1:D:362:THR:O	1:D:364:THR:HG23	2.05	0.57
1:E:173:GLU:OE1	1:E:173:GLU:N	2.38	0.57
1:B:389:ASN:ND2	1:B:391:LYS:HD3	2.15	0.57
1:D:310:ALA:HA	1:D:404:MET:CE	2.34	0.57
1:E:204:THR:HG22	1:E:224:TRP:CD1	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:245:GLU:HB3	1:E:278:LEU:HD21	1.87	0.57
1:E:259:ILE:O	1:E:260:LEU:C	2.42	0.57
1:C:256:HIS:HB3	1:C:259:ILE:HD11	1.86	0.57
1:D:466:VAL:HG21	1:D:495:LEU:HD22	1.87	0.57
1:D:299:VAL:HA	1:D:415:CYS:SG	2.44	0.57
1:E:487:ARG:NH2	1:E:490:LYS:HD2	2.14	0.57
1:D:431:LEU:CD1	1:D:450:LEU:HD13	2.35	0.57
1:E:389:ASN:ND2	1:E:391:LYS:HB3	2.19	0.57
1:D:311:SER:HA	1:D:489:LYS:HD2	1.87	0.57
1:B:437:SER:OG	1:B:440:GLU:HG3	2.05	0.57
1:C:260:LEU:HD13	1:C:340:LEU:HD12	1.87	0.57
1:D:376:LYS:HG3	1:D:379:MET:HE1	1.87	0.56
1:D:307:LEU:CA	1:D:492:LEU:HD23	2.35	0.56
1:C:406:LEU:HB3	1:C:427:PRO:HG2	1.87	0.56
1:E:445:VAL:HG13	1:E:451:ARG:NH1	2.20	0.56
1:D:456:ASN:O	1:D:459:GLN:HG2	2.05	0.56
1:D:455:PRO:HD2	1:D:458:TRP:CZ3	2.40	0.56
1:D:382:GLU:CD	1:D:482:ARG:HH22	2.08	0.56
1:A:332:ARG:NH2	1:A:373:VAL:HG11	2.21	0.56
1:B:173:GLU:N	1:B:173:GLU:OE1	2.37	0.56
1:E:256:HIS:CD2	1:E:257:GLU:N	2.73	0.56
1:C:451:ARG:HG2	1:C:475:TRP:HB3	1.87	0.56
1:B:367:ILE:HD11	1:B:371:HIS:CE1	2.40	0.56
1:E:308:SER:OG	1:E:346:THR:HG23	2.06	0.56
1:A:407:VAL:O	1:A:411:ILE:HG13	2.05	0.56
1:D:184:MET:HE3	1:D:193:LEU:HG	1.88	0.56
1:B:381:PRO:O	1:B:383:VAL:N	2.39	0.56
1:E:197:VAL:O	1:E:201:ILE:HG13	2.06	0.56
1:B:451:ARG:HE	1:B:475:TRP:HB3	1.70	0.56
1:A:313:LEU:HD21	1:A:400:ASP:HB3	1.88	0.56
1:C:199:ARG:O	1:C:203:ARG:HG3	2.05	0.56
1:E:497:GLN:C	1:E:499:GLU:H	2.09	0.56
1:D:367:ILE:CG1	1:D:369:PRO:HD3	2.24	0.56
1:A:473:GLU:HB3	1:A:483:LEU:HG	1.88	0.56
1:C:385:ASP:HA	1:C:442:ARG:HD2	1.87	0.56
1:C:356:VAL:HG23	1:C:393:PHE:HE1	1.71	0.56
1:B:216:PHE:CD2	1:B:232:LYS:HE3	2.41	0.56
1:C:430:ASP:OD1	1:C:431:LEU:HG	2.06	0.56
1:D:256:HIS:HD2	1:D:258:ASN:HB2	1.71	0.55
1:E:251:THR:O	1:E:253:MET:N	2.39	0.55
1:C:368:ALA:H	1:C:369:PRO:HD2	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:458:TRP:HB3	1:D:464:LEU:HB3	1.88	0.55
1:B:224:TRP:CH2	1:B:225:ARG:HD2	2.42	0.55
1:A:376:LYS:HE3	1:A:438:VAL:CG1	2.32	0.55
1:E:204:THR:HG22	1:E:224:TRP:HE1	1.68	0.55
1:B:381:PRO:C	1:B:383:VAL:H	2.09	0.55
1:C:367:ILE:HG23	1:C:369:PRO:CG	2.35	0.55
1:A:473:GLU:OE2	1:A:483:LEU:HD21	2.06	0.55
1:C:407:VAL:HA	1:C:410:GLU:OE2	2.06	0.55
1:A:335:LYS:O	1:A:339:ILE:HG13	2.07	0.55
1:E:310:ALA:HA	1:E:404:MET:HE3	1.89	0.55
1:B:462:GLU:O	1:B:466:VAL:HG23	2.06	0.55
1:A:413:ARG:NH1	1:A:413:ARG:HG2	2.16	0.55
1:A:470:ILE:HG23	1:A:483:LEU:HD12	1.88	0.55
1:C:303:ILE:HG21	1:C:496:SER:HB2	1.88	0.55
1:E:211:ILE:HD13	2:E:601:55F:C1	2.37	0.55
1:E:376:LYS:O	1:E:379:MET:HB2	2.07	0.55
1:E:199:ARG:HD2	1:E:203:ARG:CZ	2.35	0.55
1:B:351:ASP:OD1	2:B:601:55F:N22	2.39	0.55
1:A:234:PHE:CE1	1:A:278:LEU:HD22	2.42	0.55
1:C:385:ASP:HA	1:C:442:ARG:NE	2.22	0.55
1:A:451:ARG:HG2	1:A:475:TRP:HB3	1.89	0.55
1:C:351:ASP:C	1:C:352:LEU:HD23	2.27	0.55
1:A:301:GLY:HA2	1:A:304:LYS:NZ	2.22	0.55
1:A:473:GLU:CD	1:A:483:LEU:HD21	2.27	0.55
1:E:218:GLU:CD	1:E:220:TRP:HE1	2.10	0.55
1:A:377:ARG:C	1:A:379:MET:H	2.10	0.55
1:E:209:GLU:OE1	1:E:221:ARG:HD3	2.06	0.55
1:C:213:LYS:HD3	1:C:218:GLU:HG3	1.87	0.55
1:C:409:TRP:HZ3	1:C:425:GLN:O	1.89	0.54
1:A:388:ILE:CD1	1:A:395:SER:HB3	2.36	0.54
1:B:313:LEU:O	1:B:313:LEU:HG	2.06	0.54
1:C:402:TYR:CE1	1:C:406:LEU:HD11	2.41	0.54
1:B:188:GLY:O	1:B:189:SER:HB2	2.06	0.54
1:C:486:LEU:HD13	1:C:486:LEU:O	2.07	0.54
1:E:253:MET:CE	1:E:325:GLY:HA2	2.37	0.54
1:A:378:TYR:CD1	1:A:378:TYR:N	2.76	0.54
1:E:432:VAL:HG22	1:E:433:PRO:HD2	1.88	0.54
1:C:211:ILE:HD12	1:C:221:ARG:HB2	1.90	0.54
1:C:267:ASN:N	1:C:267:ASN:HD22	1.83	0.54
1:A:462:GLU:O	1:A:466:VAL:HG23	2.07	0.54
1:C:489:LYS:O	1:C:489:LYS:HD3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:PHE:HB2	1:C:234:PHE:CD2	2.43	0.54
1:D:424:TYR:OH	1:D:426:LEU:HD23	2.08	0.54
1:D:459:GLN:NE2	1:D:465:ARG:HH11	2.06	0.54
1:D:224:TRP:CH2	1:D:225:ARG:HD2	2.43	0.54
1:B:488:ILE:O	1:B:492:LEU:HB2	2.07	0.54
1:B:413:ARG:NH1	1:B:423:ASP:O	2.41	0.54
1:C:431:LEU:O	1:C:432:VAL:HB	2.07	0.54
1:C:441:MET:O	1:C:445:VAL:HG23	2.08	0.54
1:E:261:GLY:HA3	1:E:281:ASP:OD2	2.08	0.54
1:B:458:TRP:N	1:B:458:TRP:CD1	2.75	0.53
1:C:417:ILE:HB	1:C:420:ILE:HG12	1.90	0.53
1:C:377:ARG:HA	1:C:441:MET:CE	2.38	0.53
1:E:443:LYS:HG3	1:E:447:GLU:OE1	2.08	0.53
1:C:176:THR:O	1:C:179:ASP:HB2	2.07	0.53
1:E:410:GLU:OE1	1:E:424:TYR:OH	2.22	0.53
1:A:320:ILE:HG22	1:A:321:VAL:N	2.23	0.53
1:D:229:VAL:HG12	1:D:230:ALA:N	2.23	0.53
1:E:432:VAL:CG2	1:E:433:PRO:HD2	2.38	0.53
1:B:367:ILE:O	1:B:367:ILE:HG23	2.08	0.53
1:D:461:CYS:SG	1:D:464:LEU:HD23	2.48	0.53
1:C:382:GLU:H	1:C:382:GLU:CD	2.12	0.53
1:D:234:PHE:CE1	1:D:278:LEU:HD22	2.44	0.53
1:C:377:ARG:HE	1:C:436:PRO:CG	2.21	0.53
1:A:381:PRO:HG3	1:A:445:VAL:HG12	1.91	0.53
1:C:473:GLU:CB	1:C:483:LEU:HG	2.38	0.53
1:C:332:ARG:HE	1:C:356:VAL:CG1	2.21	0.53
1:D:331:HIS:O	1:D:332:ARG:HB2	2.08	0.53
1:E:357:ARG:HB2	1:E:366:ASP:OD2	2.08	0.53
1:C:319:GLU:HB2	1:C:328:ALA:HB2	1.91	0.53
1:A:184:MET:O	1:A:187:SER:HB3	2.09	0.53
1:C:330:ALA:HB3	1:C:356:VAL:HG22	1.90	0.53
1:A:451:ARG:HB3	1:A:475:TRP:CE3	2.44	0.53
1:D:204:THR:CG2	1:D:224:TRP:HE1	2.21	0.53
1:C:292:LEU:C	1:C:294:ARG:H	2.11	0.53
1:D:302:MET:CE	1:D:467:MET:HG3	2.39	0.53
1:A:252:VAL:HG23	1:A:253:MET:N	2.24	0.53
1:E:191:SER:HB3	1:E:252:VAL:HA	1.89	0.53
1:B:331:HIS:HD2	1:B:333:ASP:N	2.07	0.53
1:B:432:VAL:CG2	1:B:433:PRO:HD2	2.39	0.53
1:C:244:ARG:HH22	1:C:366:ASP:CG	2.12	0.52
1:B:180:LEU:HD13	1:B:201:ILE:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:494:GLN:HG3	1:C:497:GLN:NE2	2.24	0.52
1:A:443:LYS:HG2	1:A:448:GLN:HE21	1.73	0.52
1:C:454:ILE:HD12	1:C:472:ARG:CZ	2.40	0.52
1:A:397:LYS:O	1:A:400:ASP:HB2	2.09	0.52
1:B:216:PHE:CG	1:B:217:GLY:N	2.77	0.52
1:C:313:LEU:HD22	1:C:334:LEU:CD1	2.39	0.52
1:E:409:TRP:HA	1:E:471:MET:CE	2.39	0.52
1:B:365:ILE:C	1:B:367:ILE:H	2.12	0.52
1:B:204:THR:CG2	1:B:224:TRP:HE1	2.23	0.52
1:E:417:ILE:HD11	1:E:464:LEU:HD23	1.91	0.52
1:C:332:ARG:HH12	1:C:373:VAL:HB	1.75	0.52
1:D:473:GLU:HB3	1:D:483:LEU:HG	1.91	0.52
1:E:278:LEU:HD23	2:E:601:55F:H23A	1.92	0.52
1:D:388:ILE:HG23	1:D:388:ILE:O	2.09	0.52
1:A:409:TRP:CZ3	1:A:427:PRO:HA	2.45	0.52
1:B:180:LEU:CD1	1:B:201:ILE:HD11	2.39	0.52
1:E:346:THR:HG22	1:E:347:CYS:N	2.23	0.52
1:D:457:ARG:CZ	1:D:457:ARG:HB2	2.38	0.52
1:A:297:VAL:HG22	1:A:298:THR:N	2.25	0.52
1:D:451:ARG:CG	1:D:475:TRP:HB3	2.39	0.52
1:D:178:LYS:H	1:D:178:LYS:HD2	1.75	0.52
1:A:317:HIS:NE2	1:A:400:ASP:OD2	2.43	0.52
1:B:462:GLU:HA	1:B:462:GLU:OE1	2.09	0.52
1:A:413:ARG:NH1	1:A:423:ASP:O	2.43	0.52
1:D:185:THR:C	1:D:187:SER:H	2.13	0.52
1:E:216:PHE:CD1	1:E:217:GLY:N	2.78	0.51
1:E:453:ASN:O	1:E:455:PRO:HD3	2.10	0.51
1:E:389:ASN:HD21	1:E:391:LYS:CB	2.22	0.51
1:C:182:TYR:O	1:C:186:THR:HB	2.10	0.51
1:C:310:ALA:HA	1:C:404:MET:HE1	1.91	0.51
1:B:248:ILE:HD13	1:B:355:ALA:HB3	1.92	0.51
1:E:432:VAL:O	1:E:433:PRO:O	2.28	0.51
1:C:435:ASP:N	1:C:436:PRO:CD	2.72	0.51
1:C:409:TRP:HB2	1:C:471:MET:CE	2.37	0.51
1:C:354:LEU:HD22	1:C:373:VAL:HG11	1.91	0.51
1:D:466:VAL:O	1:D:470:ILE:HG13	2.11	0.51
1:B:394:GLU:O	1:B:398:ARG:HG3	2.11	0.51
1:E:208:GLN:HG2	1:E:222:GLY:HA2	1.92	0.51
1:B:244:ARG:HH11	1:B:244:ARG:HG2	1.75	0.51
1:A:313:LEU:HD11	1:A:317:HIS:NE2	2.25	0.51
1:E:417:ILE:O	1:E:420:ILE:HG12	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:285:HIS:HB3	1:E:341:VAL:CG2	2.41	0.51
1:E:256:HIS:ND1	1:E:315:HIS:CD2	2.79	0.51
1:A:470:ILE:HD11	1:A:492:LEU:HD11	1.93	0.51
1:B:409:TRP:HA	1:B:471:MET:CE	2.40	0.51
1:D:416:SER:HA	1:D:421:HIS:HB3	1.93	0.51
1:C:423:ASP:O	1:C:425:GLN:HG2	2.10	0.51
1:B:381:PRO:HD2	1:B:482:ARG:NH2	2.25	0.51
1:B:402:TYR:O	1:B:406:LEU:HD12	2.10	0.51
1:B:233:ILE:CD1	1:B:233:ILE:O	2.57	0.51
1:B:283:HIS:O	2:B:601:55F:H2	2.10	0.51
1:A:435:ASP:N	1:A:436:PRO:HD3	2.26	0.51
1:B:331:HIS:HD2	1:B:333:ASP:H	1.59	0.51
1:D:294:ARG:HD3	1:D:295:TYR:CZ	2.46	0.51
1:B:487:ARG:O	1:B:491:THR:HG23	2.11	0.51
1:A:297:VAL:HG22	1:A:298:THR:H	1.76	0.50
1:A:458:TRP:O	1:A:464:LEU:HD12	2.11	0.50
1:D:184:MET:HE2	1:D:193:LEU:HG	1.93	0.50
1:D:425:GLN:OE1	1:D:429:TYR:CD1	2.64	0.50
1:C:211:ILE:CG2	1:C:219:VAL:HG12	2.41	0.50
1:B:244:ARG:HG2	1:B:244:ARG:NH1	2.26	0.50
1:C:184:MET:O	1:C:186:THR:N	2.40	0.50
1:C:425:GLN:HB3	1:C:429:TYR:CD2	2.46	0.50
1:E:491:THR:HA	1:E:494:GLN:HG3	1.93	0.50
1:D:209:GLU:OE2	1:D:221:ARG:HD3	2.10	0.50
1:E:232:LYS:HG2	1:E:234:PHE:CE1	2.46	0.50
1:D:474:CYS:O	1:D:482:ARG:HD3	2.11	0.50
1:B:380:ALA:HB1	1:B:382:GLU:OE2	2.12	0.50
1:C:184:MET:C	1:C:186:THR:H	2.14	0.50
1:C:435:ASP:O	1:C:437:SER:N	2.45	0.50
1:E:380:ALA:HA	1:E:402:TYR:CE1	2.46	0.50
1:D:432:VAL:HG22	1:D:433:PRO:HD2	1.94	0.50
1:B:428:TYR:HD2	1:B:431:LEU:HD12	1.76	0.50
1:A:199:ARG:HD2	1:A:203:ARG:NE	2.27	0.50
1:B:389:ASN:C	1:B:391:LYS:H	2.14	0.50
1:A:195:LEU:O	1:A:198:GLN:N	2.45	0.50
1:C:341:VAL:HG23	1:C:345:GLY:O	2.11	0.50
1:A:232:LYS:HD3	1:A:234:PHE:CZ	2.47	0.50
1:C:332:ARG:HH22	1:C:373:VAL:CB	2.24	0.50
1:E:372:ARG:O	1:E:373:VAL:HG13	2.12	0.50
1:C:302:MET:HG3	1:C:411:ILE:CG2	2.39	0.50
1:D:413:ARG:NH1	1:D:423:ASP:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:240:ARG:HH11	1:D:240:ARG:CB	2.25	0.50
1:B:209:GLU:OE2	1:B:221:ARG:NH1	2.45	0.50
1:D:199:ARG:HD2	1:D:203:ARG:NH2	2.26	0.49
1:D:457:ARG:HH11	1:D:457:ARG:HB3	1.77	0.49
1:D:435:ASP:N	1:D:436:PRO:HD3	2.27	0.49
1:E:260:LEU:HD13	1:E:340:LEU:CD1	2.42	0.49
1:C:384:LEU:CD2	1:C:438:VAL:HG13	2.42	0.49
1:E:459:GLN:CA	1:E:459:GLN:HE21	2.20	0.49
1:A:377:ARG:HH12	1:A:436:PRO:HD3	1.78	0.49
1:D:268:LYS:HB2	1:D:275:GLN:HB2	1.94	0.49
1:C:182:TYR:CD1	1:E:366:ASP:HB3	2.48	0.49
1:A:489:LYS:O	1:A:493:SER:HB2	2.12	0.49
1:D:459:GLN:NE2	1:D:465:ARG:NH1	2.59	0.49
1:D:384:LEU:HB2	1:D:446:CYS:SG	2.52	0.49
1:C:417:ILE:HB	1:C:420:ILE:CG1	2.42	0.49
1:C:459:GLN:HE22	1:C:465:ARG:CG	2.23	0.49
1:E:462:GLU:O	1:E:466:VAL:HG23	2.13	0.49
1:E:310:ALA:N	1:E:404:MET:HE3	2.27	0.49
1:B:215:ARG:CG	1:B:216:PHE:H	2.26	0.49
1:A:198:GLN:HB3	1:A:264:ALA:HB1	1.95	0.49
1:B:234:PHE:CD1	1:B:234:PHE:N	2.81	0.49
1:C:377:ARG:HE	1:C:436:PRO:CD	2.26	0.49
1:D:389:ASN:HD22	1:D:389:ASN:C	2.15	0.49
1:E:385:ASP:OD2	1:E:387:SER:HB3	2.13	0.49
1:A:427:PRO:O	1:A:428:TYR:HB2	2.13	0.49
1:E:435:ASP:N	1:E:436:PRO:HD3	2.28	0.49
1:E:207:LEU:C	1:E:208:GLN:HE21	2.16	0.48
1:D:180:LEU:HD13	1:D:201:ILE:HD11	1.94	0.48
1:D:445:VAL:O	1:D:449:LYS:HA	2.12	0.48
1:D:300:GLU:OE2	1:D:301:GLY:N	2.46	0.48
1:C:245:GLU:O	1:C:249:TYR:HD1	1.95	0.48
1:B:402:TYR:O	1:B:406:LEU:CD1	2.61	0.48
1:A:455:PRO:HB2	1:A:458:TRP:CD1	2.48	0.48
1:E:388:ILE:HG12	1:E:389:ASN:N	2.28	0.48
1:D:391:LYS:HE2	1:D:392:HIS:CD2	2.48	0.48
1:B:385:ASP:O	1:B:386:ASP:C	2.51	0.48
1:D:261:GLY:HA3	1:D:281:ASP:OD2	2.12	0.48
1:A:432:VAL:HG23	1:A:440:GLU:HB3	1.94	0.48
1:A:456:ASN:C	1:A:458:TRP:H	2.17	0.48
1:C:261:GLY:O	1:C:280:SER:HB2	2.13	0.48
1:E:221:ARG:HH21	1:E:223:LYS:HE3	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:ILE:HG22	1:C:249:TYR:N	2.27	0.48
1:A:466:VAL:O	1:A:469:LYS:HB3	2.13	0.48
1:B:205:ILE:CG2	1:B:206:VAL:N	2.76	0.48
1:D:434:SER:O	1:D:435:ASP:C	2.50	0.48
1:A:331:HIS:HE1	1:A:350:ALA:O	1.97	0.48
1:E:377:ARG:HD3	1:E:427:PRO:O	2.13	0.48
1:E:204:THR:CG2	1:E:224:TRP:NE1	2.73	0.48
1:D:382:GLU:OE2	1:D:482:ARG:NH2	2.36	0.48
1:D:403:ALA:O	1:D:407:VAL:HG23	2.14	0.48
1:A:412:ALA:C	1:A:414:ARG:H	2.16	0.48
1:C:402:TYR:CZ	1:C:406:LEU:HD11	2.48	0.48
1:E:381:PRO:O	1:E:384:LEU:N	2.45	0.48
1:B:263:ILE:HG22	1:B:264:ALA:N	2.29	0.48
1:B:492:LEU:HD12	1:B:492:LEU:HA	1.62	0.48
1:E:366:ASP:O	1:E:367:ILE:HG23	2.14	0.48
1:C:320:ILE:CG2	1:C:321:VAL:N	2.76	0.48
1:E:461:CYS:SG	1:E:464:LEU:HD23	2.53	0.48
1:A:177:LEU:HB3	1:A:227:GLU:OE2	2.14	0.48
1:C:293:ASN:ND2	1:C:424:TYR:CD2	2.82	0.48
1:B:432:VAL:HG23	1:B:433:PRO:HD2	1.95	0.48
1:A:182:TYR:CD1	1:B:366:ASP:HB3	2.49	0.48
1:E:298:THR:CG2	1:E:299:VAL:N	2.77	0.47
1:E:232:LYS:HE2	1:E:234:PHE:CZ	2.49	0.47
1:B:251:THR:CG2	1:B:252:VAL:HG22	2.43	0.47
1:C:223:LYS:HA	1:C:227:GLU:O	2.15	0.47
1:C:304:LYS:HE3	1:C:304:LYS:HB2	1.63	0.47
1:B:417:ILE:O	1:B:420:ILE:HG12	2.14	0.47
1:D:409:TRP:CZ2	1:D:413:ARG:HD2	2.49	0.47
1:A:377:ARG:O	1:A:379:MET:N	2.46	0.47
1:B:473:GLU:HB2	1:B:483:LEU:CD1	2.44	0.47
1:C:458:TRP:HZ3	1:C:471:MET:SD	2.37	0.47
1:D:216:PHE:CD1	1:D:232:LYS:HE2	2.49	0.47
1:A:183:ASP:O	1:A:187:SER:HB2	2.14	0.47
1:E:394:GLU:O	1:E:398:ARG:HG3	2.14	0.47
1:C:319:GLU:CG	1:C:320:ILE:H	2.27	0.47
1:D:453:ASN:O	1:D:455:PRO:HD3	2.15	0.47
1:C:426:LEU:O	1:C:427:PRO:C	2.53	0.47
1:E:316:LEU:CD2	1:E:329:ILE:HB	2.45	0.47
1:B:389:ASN:C	1:B:391:LYS:N	2.67	0.47
1:B:389:ASN:O	1:B:391:LYS:N	2.47	0.47
1:E:497:GLN:C	1:E:499:GLU:N	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:310:ALA:CA	1:E:404:MET:HE3	2.45	0.47
1:A:301:GLY:HA2	1:A:304:LYS:HZ3	1.79	0.47
1:E:382:GLU:CD	1:E:482:ARG:HH12	2.17	0.47
1:D:417:ILE:O	1:D:420:ILE:HG12	2.14	0.47
1:A:441:MET:O	1:A:445:VAL:HG23	2.15	0.47
1:B:205:ILE:HG22	1:B:206:VAL:N	2.29	0.47
1:C:319:GLU:CG	1:C:320:ILE:N	2.77	0.47
1:E:413:ARG:NH1	1:E:422:GLU:HB3	2.30	0.47
1:D:368:ALA:CB	1:E:178:LYS:HE3	2.34	0.47
1:C:385:ASP:O	1:C:386:ASP:CB	2.63	0.47
1:B:416:SER:HA	1:B:421:HIS:HB3	1.97	0.47
1:C:242:TRP:CE3	1:C:276:LEU:HD13	2.50	0.47
1:D:211:ILE:O	1:D:211:ILE:CG2	2.62	0.47
1:A:443:LYS:HE2	1:A:448:GLN:HE22	1.79	0.47
1:A:428:TYR:CE1	1:A:452:PRO:HD3	2.50	0.47
1:A:375:THR:O	1:A:379:MET:HG3	2.14	0.47
1:C:274:THR:CG2	1:C:276:LEU:HD21	2.43	0.47
1:E:294:ARG:HD2	1:E:295:TYR:CZ	2.50	0.47
1:D:397:LYS:O	1:D:400:ASP:HB2	2.14	0.47
1:D:440:GLU:O	1:D:443:LYS:HB3	2.15	0.47
1:D:319:GLU:HB2	1:D:328:ALA:HB2	1.98	0.47
1:D:254:LEU:O	1:D:255:ARG:HB2	2.15	0.46
1:C:248:ILE:O	1:C:251:THR:HG23	2.15	0.46
1:B:420:ILE:HD12	1:B:457:ARG:HD2	1.97	0.46
1:A:257:GLU:O	1:A:257:GLU:HG2	2.15	0.46
1:E:304:LYS:NZ	1:E:304:LYS:HB2	2.31	0.46
1:E:417:ILE:HD11	1:E:464:LEU:CD2	2.44	0.46
1:E:478:ASN:HD22	1:E:479:GLY:N	2.12	0.46
1:C:432:VAL:HG11	1:C:441:MET:SD	2.55	0.46
1:E:469:LYS:O	1:E:473:GLU:HG3	2.15	0.46
1:D:235:SER:O	1:D:236:SER:C	2.54	0.46
1:C:256:HIS:O	1:C:259:ILE:N	2.45	0.46
1:D:424:TYR:CG	1:D:425:GLN:N	2.83	0.46
1:E:203:ARG:HH11	1:E:203:ARG:HG2	1.80	0.46
1:A:177:LEU:HD11	1:A:263:ILE:HD13	1.97	0.46
1:C:425:GLN:HE21	1:C:425:GLN:HA	1.81	0.46
1:D:489:LYS:O	1:D:493:SER:HB2	2.16	0.46
1:D:496:SER:C	1:D:498:GLN:H	2.19	0.46
1:D:465:ARG:CZ	1:D:465:ARG:HB2	2.45	0.46
1:A:298:THR:HG22	1:A:299:VAL:N	2.29	0.46
1:C:422:GLU:OE1	1:C:422:GLU:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:ARG:CD	1:B:203:ARG:CZ	2.93	0.46
1:C:472:ARG:C	1:C:474:CYS:H	2.18	0.46
1:B:331:HIS:HE1	1:B:350:ALA:O	1.98	0.46
1:B:434:SER:O	1:B:435:ASP:HB3	2.16	0.46
1:A:479:GLY:HA2	1:A:482:ARG:NH1	2.31	0.46
1:A:251:THR:O	1:A:253:MET:N	2.48	0.46
1:B:287:SER:HA	1:B:339:ILE:O	2.16	0.46
1:D:252:VAL:HB	1:D:324:GLN:HB2	1.98	0.46
1:C:244:ARG:NH1	1:C:367:ILE:HG13	2.31	0.46
1:C:258:ASN:C	1:C:348:CYS:HA	2.36	0.46
1:A:432:VAL:HG11	1:A:441:MET:SD	2.56	0.46
1:B:188:GLY:O	1:B:189:SER:CB	2.63	0.46
1:B:356:VAL:O	1:B:356:VAL:CG2	2.63	0.46
1:C:232:LYS:HE2	2:C:601:55F:N13	2.31	0.45
1:C:331:HIS:CD2	1:C:331:HIS:O	2.69	0.45
1:A:473:GLU:HB3	1:A:483:LEU:CD1	2.46	0.45
1:D:412:ALA:C	1:D:414:ARG:H	2.20	0.45
1:B:216:PHE:CE2	1:B:232:LYS:HE3	2.50	0.45
1:E:302:MET:CE	1:E:467:MET:HG3	2.46	0.45
1:C:479:GLY:CA	1:C:482:ARG:HD2	2.42	0.45
1:D:293:ASN:HA	1:D:293:ASN:HD22	1.58	0.45
1:C:198:GLN:HB3	1:C:264:ALA:HB1	1.98	0.45
1:A:180:LEU:HD13	1:A:201:ILE:HD11	1.98	0.45
1:C:417:ILE:HD11	1:C:464:LEU:HD21	1.97	0.45
1:C:357:ARG:H	1:C:366:ASP:HB2	1.82	0.45
1:E:368:ALA:HB3	1:E:369:PRO:CD	2.42	0.45
1:B:302:MET:HG3	1:B:411:ILE:HG22	1.98	0.45
1:C:208:GLN:HG3	1:C:221:ARG:NH1	2.30	0.45
1:C:294:ARG:HH11	1:C:294:ARG:HG2	1.81	0.45
1:C:454:ILE:HD11	1:C:475:TRP:HZ3	1.78	0.45
1:D:381:PRO:HG3	1:D:445:VAL:CG1	2.47	0.45
1:B:175:THR:HA	1:C:243:PHE:CE2	2.51	0.45
1:C:229:VAL:CG2	1:C:263:ILE:HD12	2.47	0.45
1:A:417:ILE:HG13	1:A:420:ILE:HG13	1.98	0.45
1:C:287:SER:HA	1:C:339:ILE:O	2.16	0.45
1:A:413:ARG:NH2	1:A:425:GLN:HG3	2.31	0.45
1:C:215:ARG:H	1:C:215:ARG:HE	1.62	0.45
1:C:341:VAL:O	1:C:341:VAL:HG13	2.17	0.45
1:C:408:PHE:HB3	1:C:467:MET:HE1	1.99	0.45
1:B:381:PRO:C	1:B:383:VAL:N	2.70	0.45
1:D:367:ILE:HG13	1:D:368:ALA:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:298:THR:HG22	1:C:300:GLU:N	2.11	0.45
1:C:328:ALA:C	1:C:329:ILE:HG13	2.37	0.45
1:E:409:TRP:HB2	1:E:471:MET:HE3	1.98	0.45
1:D:240:ARG:NH1	1:D:240:ARG:HB2	2.32	0.45
1:A:254:LEU:HD11	1:A:259:ILE:HG21	1.99	0.45
1:C:215:ARG:N	1:C:215:ARG:NE	2.62	0.45
1:E:442:ARG:O	1:E:446:CYS:HB2	2.17	0.45
1:A:199:ARG:HD2	1:A:203:ARG:NH2	2.31	0.45
1:E:498:GLN:C	1:E:499:GLU:HG2	2.36	0.45
1:B:256:HIS:CD2	1:B:258:ASN:H	2.34	0.45
1:A:404:MET:HG2	1:A:404:MET:O	2.17	0.44
1:A:248:ILE:CD1	1:A:355:ALA:HB3	2.46	0.44
1:B:443:LYS:HE2	1:B:448:GLN:NE2	2.33	0.44
1:C:377:ARG:HA	1:C:441:MET:HE1	1.98	0.44
1:A:409:TRP:CD1	1:A:471:MET:HE1	2.49	0.44
1:C:486:LEU:HD13	1:C:486:LEU:C	2.37	0.44
1:E:293:ASN:ND2	1:E:424:TYR:CD2	2.85	0.44
1:E:316:LEU:HD23	1:E:329:ILE:HB	2.00	0.44
1:D:313:LEU:HD13	1:D:334:LEU:HD11	1.98	0.44
1:C:216:PHE:HA	1:C:238:GLU:HG3	1.99	0.44
1:A:471:MET:O	1:A:475:TRP:CG	2.70	0.44
1:E:389:ASN:C	1:E:391:LYS:H	2.19	0.44
1:B:316:LEU:HA	1:B:316:LEU:HD23	1.89	0.44
1:D:258:ASN:O	1:D:348:CYS:HA	2.17	0.44
1:A:239:GLU:O	1:A:242:TRP:HB3	2.17	0.44
1:C:178:LYS:NZ	1:E:367:ILE:CD1	2.81	0.44
1:C:393:PHE:O	1:C:396:PHE:HB2	2.18	0.44
1:C:494:GLN:C	1:C:496:SER:H	2.20	0.44
1:E:298:THR:HG22	1:E:299:VAL:H	1.81	0.44
1:D:291:TYR:HB2	1:D:341:VAL:HG11	1.98	0.44
1:C:377:ARG:HG3	1:C:436:PRO:HG2	1.99	0.44
1:A:381:PRO:HG3	1:A:445:VAL:CG1	2.48	0.44
1:E:334:LEU:O	1:E:335:LYS:CB	2.65	0.44
1:B:331:HIS:CD2	1:B:333:ASP:H	2.36	0.44
1:A:195:LEU:O	1:A:197:VAL:N	2.51	0.44
1:C:332:ARG:HH22	1:C:373:VAL:HG21	1.82	0.44
1:B:313:LEU:HD22	1:B:334:LEU:HD11	2.00	0.44
1:A:350:ALA:O	1:A:351:ASP:CB	2.66	0.44
1:C:197:VAL:O	1:C:198:GLN:C	2.56	0.44
1:E:367:ILE:H	1:E:367:ILE:HD12	1.82	0.44
1:E:256:HIS:CD2	1:E:256:HIS:C	2.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:LEU:HD13	1:B:444:VAL:CG1	2.48	0.44
1:A:194:PRO:HB2	1:A:197:VAL:HG23	1.98	0.44
1:A:470:ILE:CA	1:A:473:GLU:HB2	2.43	0.44
1:E:334:LEU:HD23	1:E:334:LEU:HA	1.73	0.44
1:B:208:GLN:C	1:B:209:GLU:HG3	2.38	0.44
1:C:464:LEU:H	1:C:464:LEU:CD2	2.31	0.44
1:B:416:SER:HA	1:B:420:ILE:O	2.18	0.44
1:B:181:ILE:O	1:B:184:MET:HG2	2.18	0.44
1:C:331:HIS:CD2	1:C:334:LEU:N	2.86	0.43
1:C:332:ARG:HH22	1:C:373:VAL:HG11	1.83	0.43
1:B:376:LYS:HG3	1:B:379:MET:HE3	1.99	0.43
1:E:198:GLN:HE22	1:E:250:GLN:NE2	2.13	0.43
1:A:331:HIS:HD2	1:A:333:ASP:C	2.21	0.43
1:C:378:TYR:N	1:C:378:TYR:CD1	2.86	0.43
1:C:487:ARG:HH22	1:C:490:LYS:HD2	1.82	0.43
1:C:215:ARG:H	1:C:215:ARG:NE	2.16	0.43
1:A:248:ILE:HD13	1:A:355:ALA:HB3	2.00	0.43
1:A:394:GLU:O	1:A:398:ARG:HG2	2.19	0.43
1:B:234:PHE:CE1	1:B:278:LEU:HD22	2.53	0.43
1:A:409:TRP:HB2	1:A:471:MET:HE3	2.00	0.43
1:E:242:TRP:CD1	1:E:276:LEU:HB3	2.54	0.43
1:D:178:LYS:CD	1:D:178:LYS:H	2.31	0.43
1:A:375:THR:O	1:A:377:ARG:N	2.51	0.43
1:C:294:ARG:HD3	1:C:295:TYR:CZ	2.53	0.43
1:A:393:PHE:CG	1:A:393:PHE:O	2.71	0.43
1:A:428:TYR:N	1:A:428:TYR:CD1	2.86	0.43
1:E:319:GLU:OE2	1:E:360:SER:HB3	2.18	0.43
1:E:478:ASN:ND2	1:E:479:GLY:N	2.66	0.43
1:A:326:LYS:HG3	1:A:326:LYS:O	2.18	0.43
1:A:473:GLU:HB3	1:A:483:LEU:CG	2.49	0.43
1:D:451:ARG:O	1:D:452:PRO:C	2.55	0.43
1:E:409:TRP:CH2	1:E:413:ARG:HD2	2.53	0.43
1:A:431:LEU:HB3	1:A:444:VAL:HG11	2.00	0.43
1:C:224:TRP:O	1:C:225:ARG:HB2	2.18	0.43
1:C:416:SER:HA	1:C:421:HIS:HB3	2.01	0.43
1:E:178:LYS:HE2	1:E:178:LYS:HB2	1.66	0.43
1:C:468:ALA:HA	1:C:471:MET:HB2	1.99	0.43
1:A:232:LYS:HE3	2:A:601:55F:N13	2.34	0.43
1:A:470:ILE:HD13	1:A:488:ILE:HG23	1.99	0.43
1:C:428:TYR:HE2	1:C:452:PRO:CD	2.30	0.43
1:E:248:ILE:C	1:E:250:GLN:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:479:GLY:HA2	1:D:482:ARG:CZ	2.49	0.43
1:D:234:PHE:CD1	1:D:234:PHE:N	2.85	0.43
1:C:187:SER:O	1:C:189:SER:N	2.52	0.43
1:A:224:TRP:CZ3	1:A:225:ARG:HD2	2.54	0.43
1:C:362:THR:HG22	1:C:362:THR:O	2.18	0.43
1:C:186:THR:HG23	1:C:186:THR:O	2.18	0.43
1:D:214:GLY:HA3	1:D:216:PHE:CE2	2.54	0.43
1:A:431:LEU:HD13	1:A:444:VAL:CG1	2.48	0.43
1:D:380:ALA:HB1	1:D:382:GLU:OE2	2.19	0.43
1:E:376:LYS:HA	1:E:379:MET:SD	2.59	0.43
1:B:287:SER:O	1:B:288:LEU:C	2.57	0.43
1:C:425:GLN:HB3	1:C:429:TYR:CG	2.54	0.43
1:C:335:LYS:HG2	1:C:336:SER:H	1.76	0.43
1:A:224:TRP:CZ2	1:A:225:ARG:HD2	2.54	0.43
1:B:309:THR:CG2	1:B:404:MET:HE2	2.48	0.43
1:A:487:ARG:C	1:A:489:LYS:N	2.72	0.43
1:E:252:VAL:HG23	1:E:253:MET:H	1.83	0.43
1:D:200:THR:O	1:D:201:ILE:C	2.57	0.43
1:B:442:ARG:O	1:B:446:CYS:HB2	2.19	0.43
1:C:187:SER:O	1:C:188:GLY:C	2.57	0.43
1:C:299:VAL:HG21	1:C:417:ILE:HG12	2.00	0.43
1:B:381:PRO:HG3	1:B:445:VAL:CG1	2.48	0.43
1:E:450:LEU:O	1:E:451:ARG:HD3	2.19	0.43
1:C:270:ASN:O	1:C:274:THR:N	2.52	0.43
1:B:436:PRO:HB3	1:B:441:MET:HG2	2.01	0.43
1:C:389:ASN:HD22	1:C:390:MET:N	2.16	0.43
1:A:448:GLN:O	1:A:449:LYS:C	2.57	0.42
1:D:431:LEU:HD22	1:D:444:VAL:CG1	2.47	0.42
1:D:458:TRP:CG	1:D:464:LEU:HD12	2.53	0.42
1:C:380:ALA:HA	1:C:402:TYR:CE1	2.55	0.42
1:B:258:ASN:O	1:B:348:CYS:HA	2.18	0.42
1:E:263:ILE:HG22	1:E:264:ALA:N	2.34	0.42
1:C:398:ARG:HB3	1:C:482:ARG:NH1	2.30	0.42
1:D:310:ALA:CA	1:D:404:MET:HE1	2.45	0.42
1:E:305:LEU:HD22	1:E:347:CYS:SG	2.58	0.42
1:E:215:ARG:H	1:E:215:ARG:HG2	1.54	0.42
1:A:495:LEU:HD12	1:A:495:LEU:O	2.19	0.42
1:C:308:SER:O	1:C:310:ALA:N	2.53	0.42
1:C:428:TYR:HE2	1:C:452:PRO:HD3	1.84	0.42
1:A:373:VAL:HG23	1:A:374:GLY:N	2.34	0.42
1:B:292:LEU:O	1:B:414:ARG:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:HIS:C	1:A:394:GLU:H	2.22	0.42
1:D:458:TRP:O	1:D:459:GLN:CD	2.57	0.42
1:E:382:GLU:H	1:E:382:GLU:HG3	1.45	0.42
1:C:184:MET:C	1:C:186:THR:N	2.73	0.42
1:C:298:THR:O	1:C:301:GLY:N	2.50	0.42
1:A:432:VAL:CG2	1:A:440:GLU:HB3	2.50	0.42
1:C:326:LYS:HB2	1:C:327:PRO:HD2	2.01	0.42
1:A:486:LEU:O	1:A:486:LEU:HD23	2.20	0.42
1:A:252:VAL:HG23	1:A:253:MET:H	1.82	0.42
1:D:479:GLY:HA2	1:D:482:ARG:NE	2.34	0.42
1:C:175:THR:HG22	1:C:176:THR:N	2.34	0.42
1:E:302:MET:HG3	1:E:411:ILE:HG22	2.01	0.42
1:E:235:SER:O	1:E:238:GLU:N	2.50	0.42
1:C:237:ARG:O	1:C:237:ARG:HD3	2.19	0.42
1:E:252:VAL:HG23	1:E:253:MET:N	2.34	0.42
1:A:307:LEU:HD13	1:A:307:LEU:C	2.40	0.42
1:E:367:ILE:HB	1:E:370:ASN:ND2	2.35	0.42
1:C:332:ARG:O	1:C:333:ASP:HB2	2.19	0.42
1:D:432:VAL:O	1:D:433:PRO:O	2.37	0.42
1:D:306:ALA:HB1	1:D:492:LEU:HD21	2.01	0.42
1:E:462:GLU:HG2	1:E:498:GLN:HE22	1.84	0.42
1:A:412:ALA:C	1:A:414:ARG:N	2.73	0.42
1:C:312:GLY:O	1:C:315:HIS:N	2.53	0.42
1:B:254:LEU:HD11	1:B:259:ILE:HD13	2.01	0.42
1:A:420:ILE:HD12	1:A:457:ARG:NH1	2.35	0.42
1:B:178:LYS:HG2	1:C:368:ALA:CB	2.49	0.42
1:A:443:LYS:HE2	1:A:448:GLN:HE21	1.81	0.42
1:B:455:PRO:HD2	1:B:458:TRP:CE2	2.53	0.42
1:A:377:ARG:NH1	1:A:436:PRO:HD3	2.34	0.42
1:B:417:ILE:HD11	1:B:464:LEU:HD22	2.01	0.42
1:C:377:ARG:HA	1:C:441:MET:HE2	2.01	0.42
1:D:443:LYS:HG3	1:D:448:GLN:NE2	2.34	0.42
1:B:458:TRP:HZ3	1:B:471:MET:CE	2.32	0.42
1:C:311:SER:HA	1:C:489:LYS:HG3	2.01	0.42
1:C:245:GLU:HG3	1:C:249:TYR:CE1	2.54	0.42
1:B:464:LEU:HD12	1:B:464:LEU:HA	1.75	0.42
1:E:292:LEU:HA	1:E:292:LEU:HD12	1.66	0.42
1:E:311:SER:HA	1:E:489:LYS:HD2	2.01	0.42
1:A:244:ARG:HA	1:A:244:ARG:HD2	1.87	0.42
1:C:302:MET:HE1	1:C:467:MET:HG3	2.02	0.42
1:A:422:GLU:OE1	1:A:455:PRO:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:473:GLU:HG2	1:C:476:TYR:OH	2.20	0.42
1:E:423:ASP:N	1:E:423:ASP:OD2	2.42	0.42
1:D:293:ASN:ND2	1:D:424:TYR:CB	2.83	0.42
1:D:392:HIS:O	1:D:393:PHE:C	2.58	0.42
1:B:215:ARG:HG2	1:B:215:ARG:HH11	1.85	0.42
1:A:195:LEU:O	1:A:196:LEU:C	2.56	0.42
1:B:385:ASP:HB2	1:B:442:ARG:HH21	1.85	0.42
1:A:479:GLY:HA2	1:A:482:ARG:HH12	1.85	0.42
1:B:184:MET:HE3	1:B:191:SER:O	2.19	0.42
1:C:308:SER:C	1:C:310:ALA:N	2.71	0.41
1:B:444:VAL:HG13	1:B:450:LEU:HD12	2.01	0.41
1:A:252:VAL:HB	1:A:324:GLN:HB3	2.02	0.41
1:D:358:HIS:HB2	1:D:393:PHE:CD1	2.55	0.41
1:E:288:LEU:HG	1:E:292:LEU:HD22	2.01	0.41
1:C:420:ILE:CG1	1:C:420:ILE:O	2.67	0.41
1:C:289:PHE:CD2	1:C:337:LYS:HE2	2.56	0.41
1:C:459:GLN:HA	1:C:459:GLN:NE2	2.35	0.41
1:E:242:TRP:CD1	1:E:278:LEU:HD13	2.55	0.41
1:C:234:PHE:N	1:C:234:PHE:CD1	2.88	0.41
1:A:464:LEU:O	1:A:464:LEU:HD13	2.20	0.41
1:D:259:ILE:O	1:D:260:LEU:C	2.57	0.41
1:A:332:ARG:HH22	1:A:373:VAL:HG11	1.83	0.41
1:E:285:HIS:HB3	1:E:341:VAL:HG22	2.01	0.41
1:A:213:LYS:HB3	1:A:213:LYS:HE2	1.73	0.41
1:A:401:ILE:HD11	1:A:485:ALA:HB2	2.01	0.41
1:A:335:LYS:HE3	1:A:337:LYS:HB2	2.02	0.41
1:B:451:ARG:NH2	1:B:475:TRP:O	2.36	0.41
1:A:377:ARG:C	1:A:379:MET:N	2.74	0.41
1:B:435:ASP:N	1:B:436:PRO:HD3	2.35	0.41
1:C:232:LYS:HD2	1:C:234:PHE:CE1	2.55	0.41
1:A:470:ILE:H	1:A:470:ILE:HG13	1.67	0.41
1:A:489:LYS:HD3	1:A:489:LYS:C	2.41	0.41
1:C:292:LEU:C	1:C:294:ARG:N	2.74	0.41
1:A:382:GLU:OE2	1:A:482:ARG:NH2	2.44	0.41
1:C:289:PHE:HB3	1:C:337:LYS:HG2	2.03	0.41
1:C:372:ARG:CZ	1:C:438:VAL:HG21	2.50	0.41
1:C:384:LEU:O	1:C:442:ARG:HD2	2.21	0.41
1:C:327:PRO:O	1:C:329:ILE:HG13	2.20	0.41
1:D:336:SER:HB3	1:D:410:GLU:OE1	2.20	0.41
1:A:259:ILE:CD1	1:A:316:LEU:HG	2.50	0.41
1:C:237:ARG:HD3	1:C:237:ARG:C	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:LYS:HG2	3:A:9:PO4:P	2.60	0.41
1:A:234:PHE:HE1	1:A:278:LEU:HD22	1.85	0.41
1:C:354:LEU:HD23	1:C:354:LEU:HA	1.86	0.41
1:E:377:ARG:NH1	3:E:2:PO4:O1	2.40	0.41
1:A:409:TRP:CE2	1:A:452:PRO:HB3	2.56	0.41
1:B:180:LEU:HD23	1:B:180:LEU:HA	1.84	0.41
1:D:306:ALA:CB	1:D:492:LEU:HD21	2.51	0.41
1:A:487:ARG:HD2	1:A:487:ARG:HA	1.83	0.41
1:D:362:THR:O	1:D:363:ASP:C	2.59	0.41
1:E:382:GLU:OE2	1:E:482:ARG:NH1	2.49	0.41
1:D:308:SER:OG	1:D:309:THR:N	2.53	0.41
1:C:265:ALA:CB	1:C:278:LEU:HD12	2.51	0.41
1:A:315:HIS:ND1	1:A:315:HIS:O	2.53	0.41
1:A:310:ALA:HA	1:A:404:MET:HE1	2.03	0.41
1:C:336:SER:O	1:C:339:ILE:HB	2.21	0.41
1:D:376:LYS:HG3	1:D:379:MET:CE	2.50	0.41
1:C:398:ARG:O	1:C:400:ASP:N	2.54	0.41
1:C:303:ILE:HG21	1:C:496:SER:CB	2.51	0.41
1:A:367:ILE:HD12	1:A:370:ASN:CB	2.49	0.41
1:D:293:ASN:ND2	1:D:424:TYR:HB3	2.36	0.41
1:A:263:ILE:HB	1:A:279:VAL:O	2.20	0.41
1:D:244:ARG:HH11	1:D:244:ARG:HG2	1.85	0.41
1:C:451:ARG:CG	1:C:475:TRP:HB3	2.49	0.41
1:D:376:LYS:HA	1:D:379:MET:HG3	2.01	0.41
1:A:476:TYR:C	1:A:478:ASN:N	2.72	0.41
1:A:184:MET:CE	1:A:193:LEU:HG	2.51	0.41
1:D:387:SER:O	1:D:388:ILE:C	2.59	0.41
1:A:350:ALA:O	1:A:351:ASP:HB3	2.21	0.41
1:A:237:ARG:HH11	1:A:237:ARG:HB3	1.85	0.41
1:B:252:VAL:CG2	1:B:326:LYS:HA	2.43	0.41
1:A:473:GLU:HB3	1:A:483:LEU:HD11	2.03	0.41
1:E:331:HIS:CD2	1:E:331:HIS:C	2.94	0.41
1:C:452:PRO:HB2	1:C:475:TRP:CH2	2.56	0.41
1:D:414:ARG:HD2	1:D:424:TYR:HB2	2.03	0.41
1:E:356:VAL:CG2	1:E:393:PHE:HE1	2.30	0.41
1:B:385:ASP:O	1:B:387:SER:N	2.54	0.41
1:B:307:LEU:HD22	1:B:307:LEU:O	2.20	0.41
1:C:302:MET:CE	1:C:467:MET:HG3	2.50	0.40
1:A:317:HIS:ND1	1:A:397:LYS:HG2	2.36	0.40
1:D:343:LYS:HB2	3:D:13:PO4:P	2.61	0.40
1:E:443:LYS:HE2	1:E:448:GLN:HE21	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:PHE:O	1:B:238:GLU:HG3	2.21	0.40
1:D:302:MET:HE1	1:D:467:MET:HG3	2.02	0.40
1:A:342:LYS:HB3	3:A:9:PO4:O3	2.21	0.40
1:B:233:ILE:CG1	1:B:233:ILE:O	2.68	0.40
1:D:178:LYS:CD	1:D:178:LYS:N	2.83	0.40
1:A:248:ILE:C	1:A:250:GLN:N	2.74	0.40
1:A:181:ILE:O	1:A:185:THR:HG23	2.20	0.40
1:C:182:TYR:CE2	1:C:186:THR:HG21	2.56	0.40
1:C:428:TYR:N	1:C:428:TYR:CD2	2.88	0.40
1:B:376:LYS:HA	1:B:379:MET:HE2	2.01	0.40
1:E:432:VAL:HG22	1:E:433:PRO:CD	2.52	0.40
1:D:243:PHE:CD2	1:E:175:THR:HA	2.56	0.40
1:B:365:ILE:O	1:B:365:ILE:HG13	2.22	0.40
1:E:497:GLN:O	1:E:499:GLU:N	2.54	0.40
1:B:337:LYS:HD2	3:B:23:PO4:O2	2.20	0.40
1:B:194:PRO:O	1:B:197:VAL:N	2.54	0.40
1:B:300:GLU:HG3	1:B:501:ILE:HD13	2.03	0.40
1:C:333:ASP:CG	1:C:333:ASP:O	2.60	0.40
1:C:354:LEU:HD22	1:C:373:VAL:CG1	2.52	0.40
1:C:494:GLN:HG3	1:C:497:GLN:CD	2.42	0.40
1:B:431:LEU:HD22	1:B:450:LEU:HD13	2.04	0.40
1:A:331:HIS:CD2	1:A:333:ASP:C	2.95	0.40
1:B:372:ARG:NH2	1:B:438:VAL:HG11	2.36	0.40
1:A:205:ILE:HG22	1:A:206:VAL:N	2.36	0.40
1:C:432:VAL:HA	1:C:433:PRO:HD3	1.89	0.40
1:A:443:LYS:O	1:A:447:GLU:HB2	2.21	0.40
1:C:256:HIS:O	1:C:258:ASN:N	2.54	0.40
1:A:248:ILE:C	1:A:250:GLN:H	2.25	0.40
1:D:412:ALA:O	1:D:414:ARG:N	2.55	0.40
1:E:473:GLU:OE1	1:E:483:LEU:HD21	2.21	0.40
1:E:308:SER:O	1:E:309:THR:C	2.60	0.40
1:A:181:ILE:O	1:A:184:MET:HB3	2.22	0.40
1:B:487:ARG:HE	1:B:491:THR:HG22	1.86	0.40
1:E:294:ARG:HD2	1:E:295:TYR:CE1	2.57	0.40
1:E:333:ASP:HB2	1:E:354:LEU:HD12	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	324/342 (95%)	240 (74%)	61 (19%)	23 (7%)	1	12
1	B	318/342 (93%)	259 (81%)	43 (14%)	16 (5%)	3	21
1	C	328/342 (96%)	239 (73%)	61 (19%)	28 (8%)	1	8
1	D	328/342 (96%)	266 (81%)	51 (16%)	11 (3%)	5	33
1	E	328/342 (96%)	272 (83%)	37 (11%)	19 (6%)	2	17
All	All	1626/1710 (95%)	1276 (78%)	253 (16%)	97 (6%)	2	16

All (97) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	252	VAL
1	A	447	GLU
1	B	191	SER
1	B	252	VAL
1	B	386	ASP
1	C	191	SER
1	C	211	ILE
1	C	252	VAL
1	C	255	ARG
1	C	271	GLY
1	C	333	ASP
1	C	342	LYS
1	C	346	THR
1	C	376	LYS
1	C	432	VAL
1	C	433	PRO
1	D	252	VAL
1	D	255	ARG
1	D	269	ASP
1	D	388	ILE
1	D	433	PRO

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Mol	Chain	Res	Type
1	E	252	VAL
1	E	433	PRO
1	A	271	GLY
1	A	318	MET
1	A	333	ASP
1	A	376	LYS
1	A	378	TYR
1	A	393	PHE
1	A	479	GLY
1	B	188	GLY
1	B	192	GLY
1	B	382	GLU
1	C	188	GLY
1	C	386	ASP
1	C	436	PRO
1	C	458	TRP
1	E	271	GLY
1	E	322	GLY
1	E	335	LYS
1	E	351	ASP
1	A	260	LEU
1	A	386	ASP
1	A	387	SER
1	A	448	GLN
1	B	190	GLY
1	B	335	LYS
1	B	366	ASP
1	C	185	THR
1	C	186	THR
1	C	210	SER
1	C	218	GLU
1	C	366	ASP
1	C	399	ALA
1	C	484	THR
1	D	413	ARG
1	D	499	GLU
1	E	188	GLY
1	E	333	ASP
1	E	371	HIS
1	A	196	LEU
1	A	289	PHE
1	A	477	ALA

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Mol	Chain	Res	Type
1	B	189	SER
1	B	269	ASP
1	B	271	GLY
1	B	333	ASP
1	B	390	MET
1	C	257	GLU
1	C	345	GLY
1	C	455	PRO
1	D	355	ALA
1	D	386	ASP
1	E	260	LEU
1	E	336	SER
1	E	460	SER
1	E	498	GLN
1	A	188	GLY
1	A	272	THR
1	A	457	ARG
1	B	436	PRO
1	B	448	GLN
1	C	363	ASP
1	C	427	PRO
1	E	344	ASN
1	E	355	ALA
1	E	369	PRO
1	E	381	PRO
1	E	455	PRO
1	A	195	LEU
1	A	255	ARG
1	D	186	THR
1	C	327	PRO
1	E	211	ILE
1	A	454	ILE
1	D	367	ILE
1	A	455	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	281/294 (96%)	261 (93%)	20 (7%)	18	56
1	B	278/294 (95%)	252 (91%)	26 (9%)	11	39
1	C	282/294 (96%)	266 (94%)	16 (6%)	25	64
1	D	282/294 (96%)	259 (92%)	23 (8%)	14	48
1	E	282/294 (96%)	260 (92%)	22 (8%)	16	51
All	All	1405/1470 (96%)	1298 (92%)	107 (8%)	16	53

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	199	ARG
1	A	209	GLU
1	A	229	VAL
1	A	237	ARG
1	A	254	LEU
1	A	267	ASN
1	A	269	ASP
1	A	278	LEU
1	A	284	GLU
1	A	294	ARG
1	A	296	THR
1	A	334	LEU
1	A	341	VAL
1	A	378	TYR
1	A	414	ARG
1	A	428	TYR
1	A	430	ASP
1	A	464	LEU
1	A	484	THR
1	A	489	LYS
1	B	209	GLU
1	B	215	ARG
1	B	229	VAL
1	B	233	ILE
1	B	234	PHE
1	B	268	LYS
1	B	269	ASP
1	B	278	LEU
1	B	292	LEU
1	B	294	ARG
1	B	304	LYS

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Mol	Chain	Res	Type
1	B	307	LEU
1	B	316	LEU
1	B	341	VAL
1	B	351	ASP
1	B	356	VAL
1	B	362	THR
1	B	376	LYS
1	B	382	GLU
1	B	389	ASN
1	B	390	MET
1	B	406	LEU
1	B	451	ARG
1	B	464	LEU
1	B	486	LEU
1	B	491	THR
1	C	186	THR
1	C	209	GLU
1	C	215	ARG
1	C	216	PHE
1	C	241	SER
1	C	244	ARG
1	C	255	ARG
1	C	267	ASN
1	C	268	LYS
1	C	332	ARG
1	C	364	THR
1	C	389	ASN
1	C	402	TYR
1	C	415	CYS
1	C	430	ASP
1	C	483	LEU
1	D	191	SER
1	D	209	GLU
1	D	231	VAL
1	D	244	ARG
1	D	247	GLU
1	D	267	ASN
1	D	269	ASP
1	D	278	LEU
1	D	284	GLU
1	D	294	ARG
1	D	300	GLU

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Mol	Chain	Res	Type
1	D	321	VAL
1	D	371	HIS
1	D	376	LYS
1	D	377	ARG
1	D	381	PRO
1	D	382	GLU
1	D	389	ASN
1	D	429	TYR
1	D	431	LEU
1	D	457	ARG
1	D	486	LEU
1	D	491	THR
1	E	203	ARG
1	E	204	THR
1	E	215	ARG
1	E	267	ASN
1	E	278	LEU
1	E	292	LEU
1	E	294	ARG
1	E	297	VAL
1	E	307	LEU
1	E	351	ASP
1	E	366	ASP
1	E	367	ILE
1	E	376	LYS
1	E	379	MET
1	E	382	GLU
1	E	413	ARG
1	E	423	ASP
1	E	455	PRO
1	E	486	LEU
1	E	491	THR
1	E	492	LEU
1	E	499	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	250	GLN
1	A	256	HIS
1	A	258	ASN
1	A	267	ASN

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Mol	Chain	Res	Type
1	A	331	HIS
1	A	392	HIS
1	A	425	GLN
1	A	448	GLN
1	B	250	GLN
1	B	256	HIS
1	B	258	ASN
1	B	331	HIS
1	B	389	ASN
1	B	448	GLN
1	B	459	GLN
1	C	250	GLN
1	C	267	ASN
1	C	285	HIS
1	C	324	GLN
1	C	331	HIS
1	C	370	ASN
1	C	389	ASN
1	C	425	GLN
1	C	453	ASN
1	C	459	GLN
1	C	478	ASN
1	C	494	GLN
1	C	497	GLN
1	D	250	GLN
1	D	256	HIS
1	D	258	ASN
1	D	293	ASN
1	D	324	GLN
1	D	331	HIS
1	D	370	ASN
1	D	389	ASN
1	D	448	GLN
1	D	459	GLN
1	D	497	GLN
1	D	498	GLN
1	E	208	GLN
1	E	250	GLN
1	E	256	HIS
1	E	258	ASN
1	E	315	HIS
1	E	331	HIS

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Mol	Chain	Res	Type
1	E	370	ASN
1	E	389	ASN
1	E	425	GLN
1	E	448	GLN
1	E	459	GLN
1	E	478	ASN
1	E	498	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

18 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	PO4	A	21	-	4,4,4	1.15	0	6,6,6	0.27	0
3	PO4	A	26	-	4,4,4	1.13	0	6,6,6	0.27	0
2	55F	A	601	-	30,30,30	1.65	10 (33%)	30,43,43	1.63	5 (16%)
3	PO4	A	9	-	4,4,4	1.09	0	6,6,6	0.27	0
3	PO4	B	12	-	4,4,4	1.21	0	6,6,6	0.27	0
3	PO4	B	23	-	4,4,4	1.19	0	6,6,6	0.27	0
3	PO4	B	6	-	4,4,4	1.13	0	6,6,6	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	55F	B	601	-	30,30,30	1.65	9 (30%)	30,43,43	1.70	5 (16%)
3	PO4	C	10	-	4,4,4	1.06	0	6,6,6	0.27	0
2	55F	C	601	-	30,30,30	1.71	9 (30%)	30,43,43	1.62	6 (20%)
3	PO4	D	13	-	4,4,4	1.11	0	6,6,6	0.27	0
3	PO4	D	14	-	4,4,4	1.21	0	6,6,6	0.27	0
3	PO4	D	24	-	4,4,4	1.15	0	6,6,6	0.27	0
2	55F	D	601	-	30,30,30	1.67	9 (30%)	30,43,43	1.65	6 (20%)
3	PO4	E	1	-	4,4,4	1.15	0	6,6,6	0.27	0
3	PO4	E	2	-	4,4,4	1.16	0	6,6,6	0.27	0
3	PO4	E	22	-	4,4,4	1.13	0	6,6,6	0.27	0
2	55F	E	601	-	30,30,30	1.52	9 (30%)	30,43,43	1.65	6 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PO4	A	21	-	-	0/0/0/0	0/0/0/0
3	PO4	A	26	-	-	0/0/0/0	0/0/0/0
2	55F	A	601	-	-	0/7/12/12	0/4/4/4
3	PO4	A	9	-	-	0/0/0/0	0/0/0/0
3	PO4	B	12	-	-	0/0/0/0	0/0/0/0
3	PO4	B	23	-	-	0/0/0/0	0/0/0/0
3	PO4	B	6	-	-	0/0/0/0	0/0/0/0
2	55F	B	601	-	-	0/7/12/12	0/4/4/4
3	PO4	C	10	-	-	0/0/0/0	0/0/0/0
2	55F	C	601	-	-	0/7/12/12	0/4/4/4
3	PO4	D	13	-	-	0/0/0/0	0/0/0/0
3	PO4	D	14	-	-	0/0/0/0	0/0/0/0
3	PO4	D	24	-	-	0/0/0/0	0/0/0/0
2	55F	D	601	-	-	0/7/12/12	0/4/4/4
3	PO4	E	1	-	-	0/0/0/0	0/0/0/0
3	PO4	E	2	-	-	0/0/0/0	0/0/0/0
3	PO4	E	22	-	-	0/0/0/0	0/0/0/0
2	55F	E	601	-	-	0/7/12/12	0/4/4/4

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	55F	C14-N13	-3.51	1.28	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	601	55F	C9-C11	-2.76	1.46	1.49
2	B	601	55F	C14-N13	-2.70	1.30	1.34
2	C	601	55F	C9-C11	-2.68	1.46	1.49
2	A	601	55F	C9-C11	-2.65	1.46	1.49
2	E	601	55F	C14-N13	-2.59	1.30	1.34
2	C	601	55F	C14-N13	-2.52	1.30	1.34
2	A	601	55F	C14-N13	-2.46	1.30	1.34
2	B	601	55F	C9-C11	-2.22	1.46	1.49
2	D	601	55F	C14-N22	-2.05	1.36	1.39
2	C	601	55F	C5-C4	2.01	1.46	1.42
2	A	601	55F	C8-C9	2.01	1.43	1.39
2	A	601	55F	C5-C4	2.03	1.46	1.42
2	E	601	55F	C20-N21	2.08	1.37	1.34
2	D	601	55F	C14-N15	2.08	1.37	1.34
2	A	601	55F	C16-N21	2.09	1.37	1.34
2	B	601	55F	C14-N15	2.12	1.37	1.34
2	A	601	55F	C25-N22	2.17	1.39	1.36
2	C	601	55F	C19-C20	2.18	1.41	1.38
2	E	601	55F	C16-N21	2.21	1.38	1.34
2	E	601	55F	C1-N6	2.23	1.37	1.32
2	E	601	55F	C2-N3	2.24	1.37	1.32
2	D	601	55F	C2-N3	2.42	1.37	1.32
2	A	601	55F	C2-N3	2.48	1.37	1.32
2	C	601	55F	C1-N6	2.50	1.37	1.32
2	E	601	55F	C25-N22	2.50	1.40	1.36
2	C	601	55F	C20-N21	2.51	1.38	1.34
2	B	601	55F	C1-N6	2.57	1.37	1.32
2	E	601	55F	C7-C8	2.57	1.42	1.36
2	B	601	55F	C25-N22	2.62	1.40	1.36
2	D	601	55F	C7-C8	2.64	1.42	1.36
2	D	601	55F	C19-C20	2.65	1.41	1.38
2	A	601	55F	C1-N6	2.65	1.37	1.32
2	D	601	55F	C1-N6	2.74	1.38	1.32
2	A	601	55F	C7-C8	2.76	1.42	1.36
2	B	601	55F	C2-N3	2.79	1.38	1.32
2	E	601	55F	C14-N15	2.80	1.38	1.34
2	D	601	55F	C16-N21	2.81	1.38	1.34
2	B	601	55F	C16-N21	2.84	1.38	1.34
2	D	601	55F	C20-N21	2.86	1.38	1.34
2	B	601	55F	C7-C8	2.86	1.42	1.36
2	C	601	55F	C2-N3	2.88	1.38	1.32
2	C	601	55F	C7-C8	2.93	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	55F	C20-N21	2.95	1.38	1.34
2	A	601	55F	C20-N21	3.02	1.38	1.34
2	C	601	55F	C16-N21	3.13	1.39	1.34

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	55F	C14-N22-C25	-4.74	122.80	130.17
2	D	601	55F	C14-N22-C25	-4.64	122.95	130.17
2	C	601	55F	C14-N22-C25	-4.39	123.33	130.17
2	E	601	55F	C14-N22-C25	-4.38	123.36	130.17
2	B	601	55F	C14-N22-C25	-4.05	123.88	130.17
2	D	601	55F	C12-C11-N15	-3.98	103.02	113.76
2	B	601	55F	C12-C11-N15	-3.85	103.38	113.76
2	C	601	55F	C12-C11-N15	-3.78	103.56	113.76
2	E	601	55F	C12-C11-N15	-3.76	103.61	113.76
2	A	601	55F	C12-C11-N15	-3.74	103.68	113.76
2	B	601	55F	C27-C25-N22	-2.76	111.03	114.97
2	E	601	55F	C27-C25-N22	-2.69	111.14	114.97
2	D	601	55F	C27-C25-N22	-2.65	111.19	114.97
2	A	601	55F	C27-C25-N22	-2.54	111.35	114.97
2	C	601	55F	C27-C25-N22	-2.51	111.39	114.97
2	D	601	55F	C18-C19-C20	-2.33	118.81	124.08
2	B	601	55F	C18-C19-C20	-2.17	119.17	124.08
2	A	601	55F	C18-C19-C20	-2.14	119.24	124.08
2	C	601	55F	C18-C19-C20	-2.10	119.33	124.08
2	E	601	55F	C18-C19-C20	-2.03	119.49	124.08
2	E	601	55F	C10-C5-N6	2.03	120.20	117.95
2	C	601	55F	C10-C5-N6	2.04	120.21	117.95
2	D	601	55F	C10-C5-N6	2.38	120.58	117.95
2	D	601	55F	O26-C25-N22	4.18	128.12	123.13
2	A	601	55F	O26-C25-N22	4.49	128.49	123.13
2	C	601	55F	O26-C25-N22	4.58	128.59	123.13
2	E	601	55F	O26-C25-N22	4.78	128.83	123.13
2	B	601	55F	O26-C25-N22	5.02	129.12	123.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	55F	1	0
3	A	9	PO4	2	0
3	B	23	PO4	1	0
2	B	601	55F	2	0
2	C	601	55F	1	0
3	D	13	PO4	2	0
3	E	2	PO4	2	0
2	E	601	55F	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	328/342 (95%)	0.17	11 (3%) 49 49	31, 89, 131, 142	0
1	B	324/342 (94%)	-0.13	0 100 100	27, 51, 84, 105	0
1	C	330/342 (96%)	0.59	42 (12%) 5 4	28, 101, 138, 144	0
1	D	330/342 (96%)	-0.09	3 (0%) 85 87	31, 58, 97, 109	0
1	E	330/342 (96%)	-0.08	3 (0%) 85 87	26, 51, 86, 109	0
All	All	1642/1710 (96%)	0.09	59 (3%) 46 46	26, 63, 128, 144	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	491	THR	5.7
1	C	496	SER	5.0
1	C	495	LEU	4.8
1	C	322	GLY	4.6
1	E	369	PRO	4.3
1	E	368	ALA	4.2
1	C	427	PRO	4.1
1	D	446	CYS	3.6
1	C	434	SER	3.6
1	C	420	ILE	3.5
1	C	474	CYS	3.5
1	C	416	SER	3.4
1	C	432	VAL	3.3
1	C	447	GLU	3.3
1	C	492	LEU	3.3
1	C	458	TRP	3.2
1	A	424	TYR	3.2
1	C	425	GLN	3.2
1	C	321	VAL	3.1
1	C	436	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	424	TYR	3.0
1	C	380	ALA	3.0
1	A	440	GLU	3.0
1	C	456	ASN	3.0
1	D	324	GLN	2.9
1	C	431	LEU	2.9
1	C	383	VAL	2.9
1	C	452	PRO	2.8
1	C	385	ASP	2.8
1	C	446	CYS	2.8
1	A	428	TYR	2.7
1	A	433	PRO	2.7
1	A	323	THR	2.7
1	C	323	THR	2.6
1	C	498	GLN	2.6
1	C	302	MET	2.6
1	C	409	TRP	2.5
1	A	322	GLY	2.5
1	C	467	MET	2.5
1	E	324	GLN	2.5
1	C	415	CYS	2.4
1	C	295	TYR	2.4
1	C	433	PRO	2.4
1	C	406	LEU	2.4
1	C	296	THR	2.3
1	C	376	LYS	2.3
1	C	463	ALA	2.3
1	C	439	GLU	2.3
1	A	324	GLN	2.2
1	C	455	PRO	2.2
1	D	190	GLY	2.2
1	A	500	GLY	2.2
1	C	462	GLU	2.1
1	C	426	LEU	2.1
1	A	294	ARG	2.1
1	A	427	PRO	2.1
1	C	468	ALA	2.1
1	C	482	ARG	2.0
1	A	464	LEU	2.0



## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	PO4	D	14	5/5	0.93	0.40	4.76	21,22,22,23	5
3	PO4	D	24	5/5	0.93	0.29	2.42	29,29,31,31	5
3	PO4	B	12	5/5	0.92	0.33	2.10	20,21,22,23	5
2	55F	E	601	27/27	0.95	0.27	1.64	36,40,59,62	0
2	55F	D	601	27/27	0.96	0.26	1.32	48,49,58,61	0
3	PO4	B	23	5/5	0.93	0.25	1.31	31,31,32,32	5
3	PO4	C	10	5/5	0.88	0.30	1.30	103,104,104,105	0
3	PO4	E	2	5/5	0.95	0.29	1.22	7,8,8,9	5
2	55F	A	601	27/27	0.95	0.28	0.64	46,53,65,67	0
3	PO4	E	1	5/5	0.93	0.24	0.61	89,89,90,90	0
2	55F	B	601	27/27	0.96	0.23	0.56	29,39,49,52	0
2	55F	C	601	27/27	0.91	0.26	0.47	73,79,81,81	0
3	PO4	E	22	5/5	0.95	0.21	0.04	18,18,20,20	5
3	PO4	A	26	5/5	0.93	0.24	-0.56	48,48,48,49	5
3	PO4	A	21	5/5	0.91	0.20	-1.20	36,36,37,38	5
3	PO4	B	6	5/5	0.96	0.13	-2.05	60,63,63,65	0
3	PO4	D	13	5/5	0.95	0.12	-2.30	82,82,83,84	0
3	PO4	A	9	5/5	0.88	0.17	-	103,103,104,104	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.