



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:58 AM GMT

PDB ID : 3KCF  
Title : Crystal structure of TGFbRI complexed with a pyrazolone inhibitor  
Authors : Boriack-Sjodin, P.A.  
Deposited on : 2009-10-21  
Resolution : 2.80 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

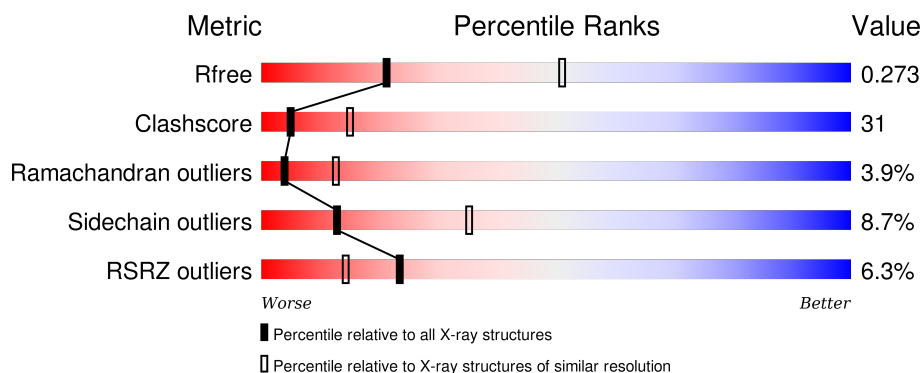
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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>8%</div> <div>45%</div> <div>44%</div> <div>6%</div> <div>.</div> </div>
1	B	342	<div> <div>2%</div> <div>51%</div> <div>38%</div> <div>6%</div> <div>5%</div> </div>
1	C	342	<div> <div>12%</div> <div>37%</div> <div>51%</div> <div>8%</div> <div>.</div> </div>
1	D	342	<div> <div>4%</div> <div>52%</div> <div>38%</div> <div>6%</div> <div>.</div> </div>
1	E	342	<div> <div>4%</div> <div>54%</div> <div>35%</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	B	11	-	-	X	-
3	PO4	D	14	-	-	-	X
3	PO4	D	15	-	-	X	X
3	PO4	E	2	-	-	X	X
3	PO4	E	3	-	-	X	-

## 2 Entry composition [i](#)

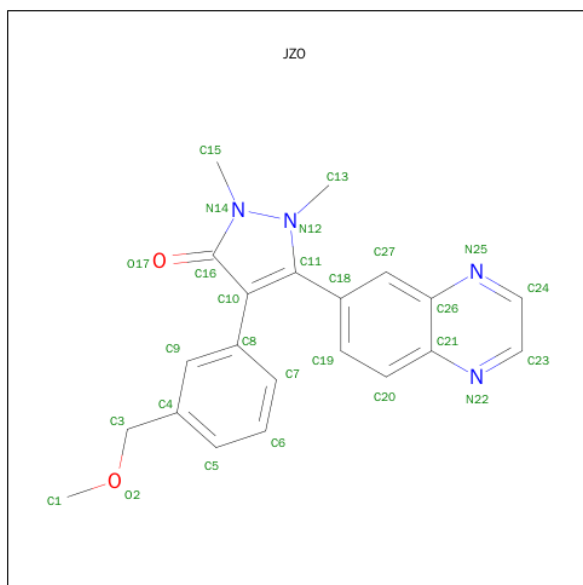
There are 4 unique types of molecules in this entry. The entry contains 13297 atoms, of which 0 are hydrogens and 0 are deuteriums.

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			

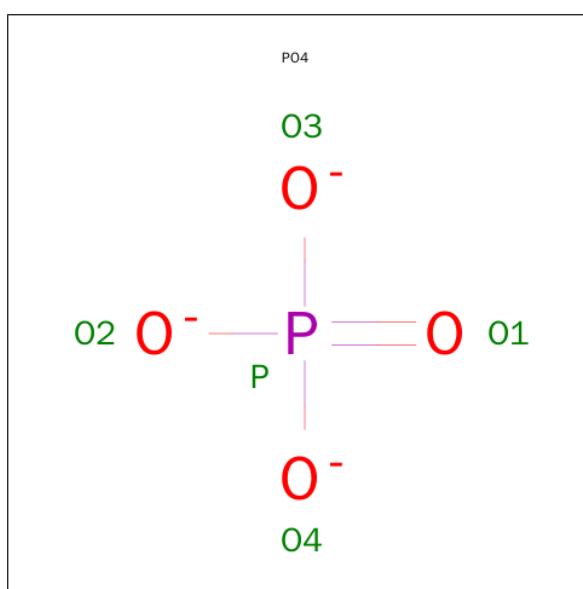
- Molecule 2 is 4-[3-(METHOXYMETHYL)PHENYL]-1,2-DIMETHYL-5-QUINOXALIN-6-YL-1,2-DIHYDRO-3H-PYRAZOL-3-ONE (three-letter code: JZO) (formula: C<sub>21</sub>H<sub>20</sub>N<sub>4</sub>O<sub>2</sub>).



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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			27	21	4	2		
2	C	1	Total	C	N	O	0	0
			27	21	4	2		
2	D	1	Total	C	N	O	0	0
			27	21	4	2		
2	E	1	Total	C	N	O	0	0
			27	21	4	2		

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



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

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

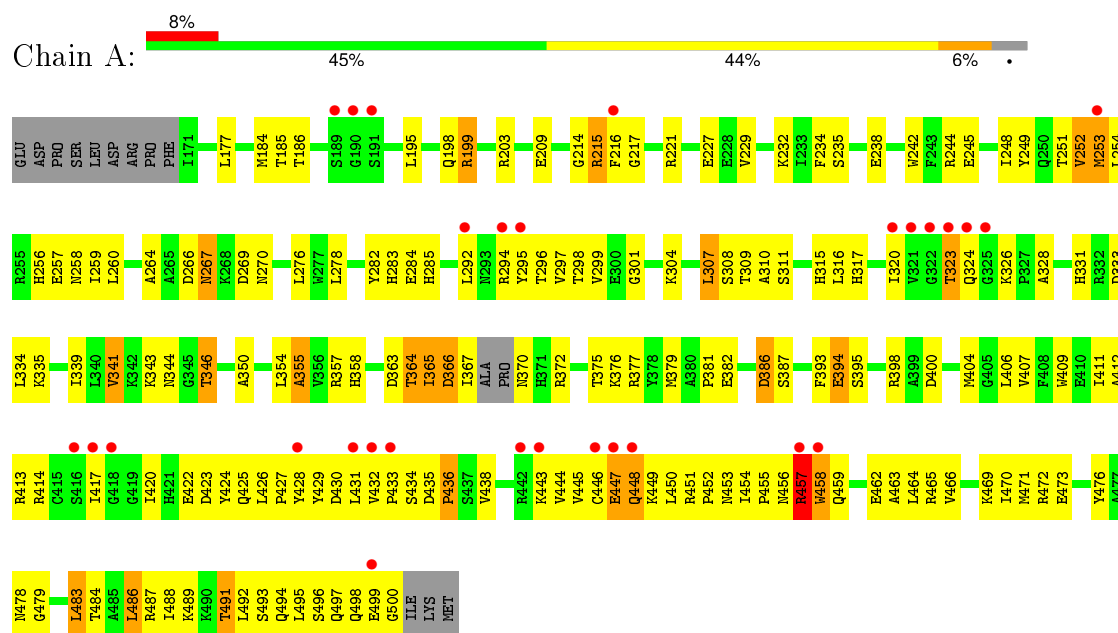
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	C	1	Total	O	0	0
			1	1		
4	E	1	Total	O	0	0
			1	1		

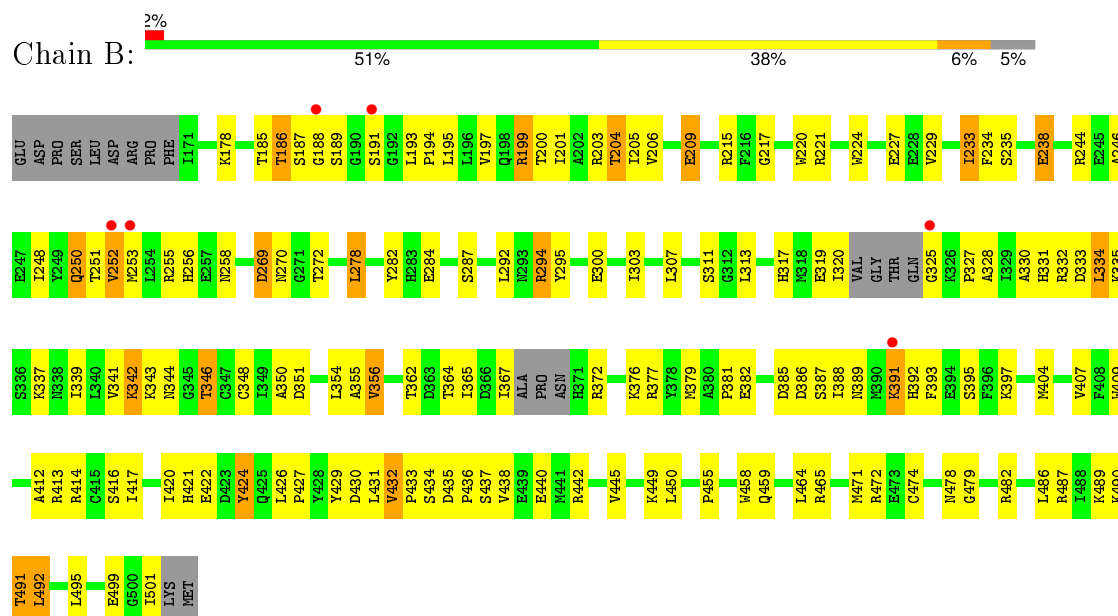
### 3 Residue-property plots

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.

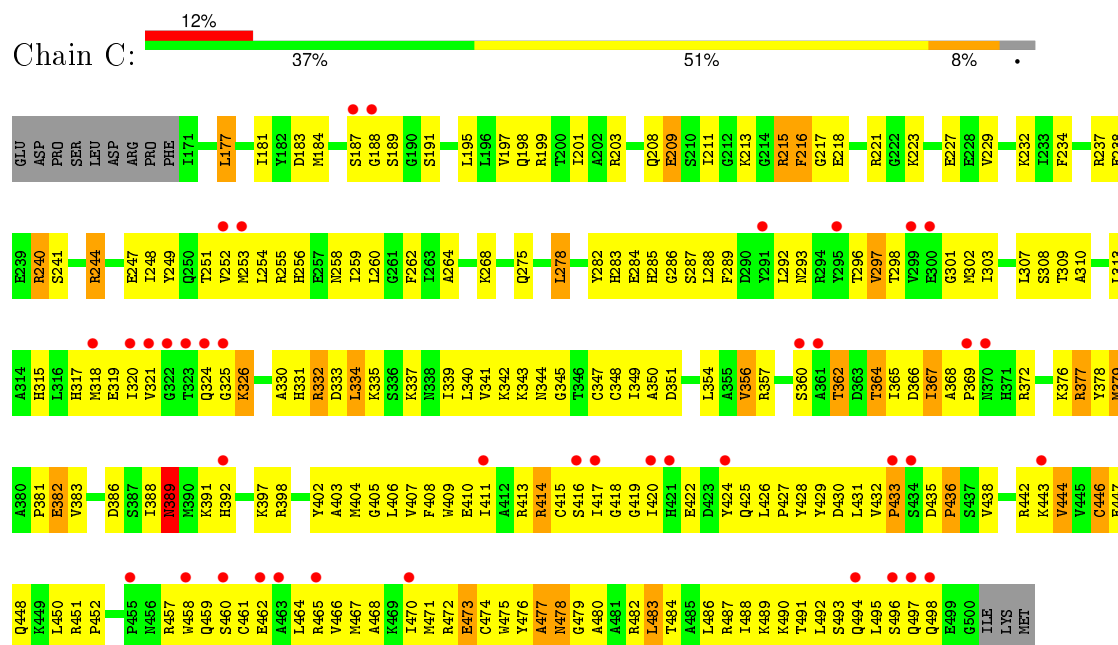
#### • Molecule 1: TGF-beta receptor type-1



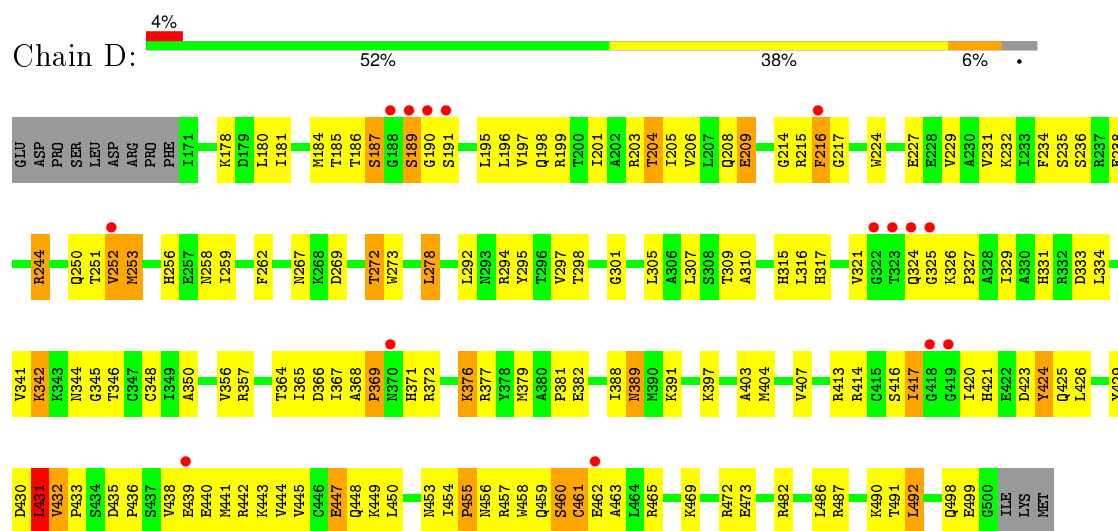
#### • Molecule 1: TGF-beta receptor type-1



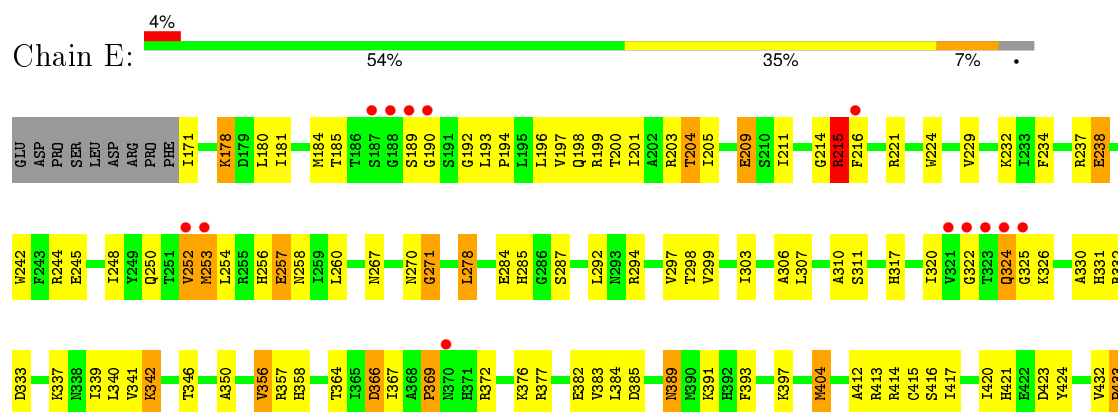
• Molecule 1: TGF-beta receptor type-1



• Molecule 1: TGF-beta receptor type-1



• Molecule 1: TGF-beta receptor type-1



S434	D435	P436	S437	E440	Y441	R442	R443	Y444	Y445	C446	E447	Q448	R449	L450	R451	I454	P455	I456	R457	Y458	Q459	S460	C461	L464	R465	Y466	Y467	Y471	R472	E473	G479	R482	L483	R487	I488	R489	R490	Y491	L492	S493	Q494	Q497	Q498	E499	G500	ILE	LYS	MEI
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## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	174.03Å 249.08Å 138.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.86 – 2.80 49.59 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (34.86-2.80) 99.7 (49.59-2.80)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.12 (at 2.81Å)	Xtriage
Refinement program	CNX 2005	Depositor
R, $R_{free}$	0.235 , 0.278 0.232 , 0.273	Depositor DCC
$R_{free}$ test set	3747 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.2	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 65.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 73507 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	13297	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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

### 5.1 Standard geometry

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

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	1/2668 (0.0%)	0.58	0/3600
1	B	0.40	0/2640	0.65	0/3560
1	C	0.34	0/2682	0.61	0/3622
1	D	0.39	0/2682	0.69	0/3622
1	E	0.41	0/2682	0.67	0/3622
All	All	0.38	1/13354 (0.0%)	0.64	0/18026

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	1
1	E	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	245	GLU	N-CA	5.55	1.57	1.46

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	424	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	D	424	TYR	Sidechain
1	E	424	TYR	Sidechain

## 5.2 Too-close contacts

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	170	0
1	B	2590	0	2595	119	0
1	C	2629	0	2631	251	0
1	D	2629	0	2631	151	0
1	E	2629	0	2631	132	0
2	A	27	0	20	1	0
2	B	27	0	20	0	0
2	C	27	0	20	3	0
2	D	27	0	20	3	0
2	E	27	0	20	1	0
3	A	15	0	0	0	0
3	B	15	0	0	4	0
3	C	5	0	0	1	0
3	D	15	0	0	2	0
3	E	15	0	0	4	0
4	A	1	0	0	1	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
All	All	13297	0	13206	823	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 31.

All (823) 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:E:216:PHE:HB3	1:E:238:GLU:HG2	1.22	1.10
1:A:443:LYS:HG2	1:A:448:GLN:HE21	1.19	1.08
1:C:461:CYS:HB2	1:C:464:LEU:HD23	1.35	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:367:ILE:HG13	1:D:369:PRO:HD3	1.40	1.04
1:E:253:MET:HB2	1:E:326:LYS:HB3	1.41	1.01
1:E:367:ILE:HG13	1:E:369:PRO:HD3	1.40	1.01
1:C:253:MET:HB3	1:C:326:LYS:HB3	1.49	0.95
1:E:256:HIS:HD2	1:E:258:ASN:H	1.11	0.94
1:C:244:ARG:HH11	1:C:367:ILE:HG12	1.33	0.93
1:B:331:HIS:HD2	1:B:333:ASP:H	1.17	0.92
1:C:215:ARG:HH11	1:C:215:ARG:HB3	1.33	0.91
1:D:417:ILE:HG13	1:D:420:ILE:HG13	1.49	0.91
1:A:372:ARG:HH11	1:A:438:VAL:HG11	1.33	0.91
1:B:317:HIS:HB3	1:B:397:LYS:HE3	1.53	0.88
1:C:376:LYS:HA	1:C:379:MET:HG3	1.56	0.87
1:C:417:ILE:HB	1:C:420:ILE:HD11	1.57	0.86
1:A:443:LYS:HG2	1:A:448:GLN:NE2	1.88	0.86
1:C:406:LEU:HD12	1:C:427:PRO:HB3	1.58	0.86
1:E:487:ARG:O	1:E:491:THR:HG22	1.76	0.86
1:E:216:PHE:HB3	1:E:238:GLU:CG	2.06	0.86
1:A:267:ASN:H	1:A:267:ASN:HD22	1.20	0.86
1:A:372:ARG:HH21	1:A:386:ASP:HB2	1.39	0.85
1:A:267:ASN:N	1:A:267:ASN:HD22	1.74	0.84
1:D:487:ARG:NH2	1:D:490:LYS:HD2	1.92	0.84
1:C:215:ARG:HG3	1:C:216:PHE:H	1.41	0.83
1:A:498:GLN:HG3	1:A:499:GLU:H	1.44	0.81
1:D:253:MET:HE2	1:D:324:GLN:O	1.80	0.81
1:E:204:THR:HG22	1:E:224:TRP:NE1	1.96	0.80
1:D:251:THR:O	1:D:252:VAL:HG22	1.81	0.80
1:B:244:ARG:HH11	1:B:244:ARG:HG2	1.46	0.80
1:D:389:ASN:ND2	1:D:391:LYS:H	1.79	0.79
1:C:244:ARG:NH1	1:C:367:ILE:HG12	1.97	0.78
1:A:309:THR:HG22	1:A:404:MET:HE2	1.64	0.78
1:A:259:ILE:HD11	1:A:316:LEU:HG	1.66	0.78
1:C:199:ARG:HD2	1:C:203:ARG:CZ	2.14	0.78
1:A:372:ARG:NH2	1:A:386:ASP:HB2	1.97	0.78
1:A:457:ARG:HH11	1:A:457:ARG:HB2	1.49	0.78
1:E:256:HIS:CD2	1:E:258:ASN:H	1.98	0.77
1:D:469:LYS:O	1:D:473:GLU:HG3	1.85	0.77
1:D:487:ARG:HH22	1:D:490:LYS:HD2	1.48	0.76
1:A:417:ILE:HG13	1:A:420:ILE:HD11	1.66	0.76
1:D:252:VAL:HG21	1:D:327:PRO:HD2	1.66	0.75
1:E:204:THR:HG22	1:E:224:TRP:HE1	1.47	0.75
1:A:301:GLY:HA2	1:A:304:LYS:NZ	2.02	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:LYS:HA	1:A:379:MET:SD	2.27	0.74
1:D:389:ASN:HD21	1:D:391:LYS:HB3	1.51	0.74
1:C:479:GLY:HA2	1:C:482:ARG:HD2	1.69	0.74
1:D:317:HIS:HB3	1:D:397:LYS:HE3	1.70	0.74
1:E:357:ARG:HB2	1:E:366:ASP:HB2	1.68	0.74
1:C:297:VAL:HG22	1:C:298:THR:H	1.50	0.74
1:A:455:PRO:O	1:A:458:TRP:HB2	1.87	0.74
1:E:199:ARG:HD2	1:E:203:ARG:CZ	2.19	0.73
1:B:256:HIS:CD2	1:B:258:ASN:H	2.05	0.73
1:B:344:ASN:OD1	1:B:346:THR:HB	1.88	0.73
1:D:331:HIS:HD2	1:D:333:ASP:H	1.36	0.73
1:C:432:VAL:HG21	1:C:436:PRO:HB3	1.71	0.73
1:C:320:ILE:HG22	1:C:321:VAL:H	1.55	0.72
1:D:198:GLN:HE22	1:D:250:GLN:HE21	1.38	0.72
1:A:249:TYR:HA	1:A:254:LEU:HD23	1.71	0.72
1:C:249:TYR:HA	1:C:254:LEU:HD23	1.72	0.72
1:A:284:GLU:HB3	1:A:343:LYS:HE2	1.73	0.71
1:D:435:ASP:HA	3:D:15:PO4:O3	1.90	0.71
1:E:256:HIS:HD2	1:E:258:ASN:N	1.89	0.71
1:E:417:ILE:O	1:E:420:ILE:HG12	1.91	0.71
1:C:473:GLU:HB3	1:C:483:LEU:HG	1.73	0.71
1:C:406:LEU:HD12	1:C:427:PRO:CB	2.21	0.70
1:C:199:ARG:HD2	1:C:203:ARG:NH2	2.07	0.70
1:D:199:ARG:HD2	1:D:203:ARG:CZ	2.21	0.70
1:D:414:ARG:HH21	1:D:423:ASP:HA	1.55	0.70
1:D:256:HIS:CD2	1:D:258:ASN:H	2.09	0.70
1:A:498:GLN:HG3	1:A:499:GLU:N	2.06	0.70
1:C:461:CYS:CB	1:C:464:LEU:HD23	2.17	0.69
1:C:483:LEU:HD13	1:C:488:ILE:HD11	1.74	0.69
1:E:356:VAL:HG22	1:E:393:PHE:HE1	1.57	0.69
1:A:307:LEU:HD23	1:A:492:LEU:HB3	1.74	0.69
1:C:444:VAL:HG13	1:C:450:LEU:HD12	1.74	0.69
1:C:240:ARG:HB2	1:C:240:ARG:HH11	1.57	0.69
1:C:253:MET:HB3	1:C:326:LYS:CB	2.20	0.69
1:D:357:ARG:HB2	1:D:366:ASP:HB2	1.74	0.69
1:C:414:ARG:HB3	1:C:414:ARG:HH11	1.57	0.69
1:C:320:ILE:HG22	1:C:321:VAL:N	2.07	0.69
1:C:376:LYS:HA	1:C:379:MET:CG	2.20	0.69
1:B:252:VAL:HG12	1:B:253:MET:HG3	1.75	0.69
1:D:389:ASN:HD22	1:D:389:ASN:C	1.97	0.68
1:A:309:THR:HG22	1:A:404:MET:CE	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:252:VAL:HG12	1:E:253:MET:H	1.58	0.68
1:E:467:MET:O	1:E:471:MET:HG3	1.93	0.68
1:E:253:MET:HG3	1:E:326:LYS:N	2.09	0.68
1:A:469:LYS:O	1:A:473:GLU:HG3	1.94	0.68
1:C:459:GLN:NE2	1:C:465:ARG:HG3	2.09	0.68
1:C:381:PRO:HD2	1:C:482:ARG:HH22	1.58	0.68
1:C:470:ILE:HD13	1:C:488:ILE:HG23	1.76	0.67
1:A:367:ILE:O	1:A:370:ASN:HB2	1.94	0.67
1:B:376:LYS:HA	1:B:379:MET:CE	2.24	0.67
1:E:331:HIS:HD2	1:E:333:ASP:H	1.42	0.67
1:A:267:ASN:ND2	1:A:267:ASN:N	2.42	0.67
1:A:443:LYS:HE2	1:A:448:GLN:NE2	2.11	0.66
1:C:414:ARG:HH11	1:C:414:ARG:CB	2.09	0.66
1:C:215:ARG:HG3	1:C:216:PHE:N	2.11	0.66
1:D:178:LYS:N	1:D:178:LYS:HD3	2.08	0.66
1:C:215:ARG:HH11	1:C:215:ARG:CB	2.07	0.66
1:B:431:LEU:O	1:B:432:VAL:HG23	1.96	0.66
1:A:235:SER:HB2	1:A:238:GLU:HG2	1.78	0.66
1:A:372:ARG:NH1	1:A:438:VAL:HG11	2.10	0.66
1:B:385:ASP:HA	1:B:442:ARG:CZ	2.26	0.66
1:B:376:LYS:HA	1:B:379:MET:HE3	1.78	0.66
1:E:189:SER:O	1:E:252:VAL:HG13	1.96	0.65
1:E:260:LEU:HD13	1:E:340:LEU:HD13	1.78	0.65
1:C:414:ARG:HB3	1:C:414:ARG:NH1	2.11	0.65
1:A:284:GLU:OE2	1:A:343:LYS:HE2	1.96	0.65
1:D:389:ASN:HD22	1:D:391:LYS:H	1.43	0.65
1:E:258:ASN:ND2	1:E:311:SER:HB2	2.12	0.65
1:C:357:ARG:NE	1:C:366:ASP:OD1	2.28	0.65
1:A:458:TRP:O	1:A:464:LEU:HD12	1.97	0.65
1:C:430:ASP:OD1	1:C:431:LEU:HG	1.95	0.65
1:C:372:ARG:NH1	1:C:438:VAL:HG11	2.11	0.65
1:D:251:THR:HG22	1:D:252:VAL:HG13	1.79	0.65
1:A:394:GLU:O	1:A:398:ARG:HG2	1.97	0.65
1:E:297:VAL:HG12	1:E:298:THR:O	1.97	0.64
1:D:443:LYS:HA	1:D:447:GLU:CG	2.27	0.64
1:E:204:THR:CG2	1:E:224:TRP:HE1	2.09	0.64
1:D:235:SER:O	1:D:238:GLU:HG2	1.97	0.64
1:E:253:MET:HB2	1:E:326:LYS:CB	2.25	0.64
1:A:217:GLY:N	1:A:238:GLU:OE2	2.31	0.64
1:A:298:THR:HG22	1:A:299:VAL:N	2.11	0.64
1:A:463:ALA:HB1	1:A:495:LEU:HD21	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:262:PHE:HD1	2:D:4:JZO:H1	1.63	0.64
1:E:244:ARG:NH2	1:E:366:ASP:OD2	2.30	0.64
1:C:331:HIS:HD2	1:C:333:ASP:H	1.44	0.64
1:E:322:GLY:HA3	1:E:324:GLN:NE2	2.13	0.64
1:B:244:ARG:HG2	1:B:244:ARG:NH1	2.11	0.64
1:C:490:LYS:O	1:C:494:GLN:HB2	1.98	0.64
1:A:445:VAL:O	1:A:449:LYS:HA	1.98	0.64
1:C:237:ARG:HD3	1:C:238:GLU:OE2	1.98	0.63
1:C:467:MET:O	1:C:471:MET:HG3	1.99	0.63
1:C:309:THR:HG22	1:C:404:MET:HE2	1.80	0.63
1:D:367:ILE:CG1	1:D:369:PRO:HD3	2.23	0.63
1:B:381:PRO:HG3	1:B:445:VAL:CG1	2.28	0.63
1:C:418:GLY:O	1:C:420:ILE:N	2.31	0.63
1:E:357:ARG:H	1:E:366:ASP:HB3	1.63	0.63
1:B:204:THR:CG2	1:B:224:TRP:HE1	2.12	0.63
1:C:418:GLY:O	1:C:420:ILE:HG23	1.99	0.62
1:C:368:ALA:N	1:C:369:PRO:HD2	2.14	0.62
1:E:445:VAL:HG13	1:E:451:ARG:NH1	2.14	0.62
1:A:454:ILE:HG23	1:A:458:TRP:CE3	2.34	0.62
1:B:215:ARG:HD2	1:B:351:ASP:OD2	2.00	0.62
1:A:301:GLY:HA2	1:A:304:LYS:HZ2	1.64	0.62
1:E:199:ARG:HD2	1:E:203:ARG:NH2	2.15	0.62
1:C:459:GLN:HA	1:C:459:GLN:HE21	1.63	0.62
1:A:298:THR:HG22	1:A:299:VAL:H	1.63	0.62
1:D:244:ARG:NH2	1:D:367:ILE:HG22	2.14	0.62
1:C:285:HIS:HB2	1:C:341:VAL:HG13	1.81	0.62
1:C:297:VAL:HG12	1:C:415:CYS:HA	1.81	0.62
1:E:184:MET:HB3	1:E:193:LEU:HD23	1.82	0.62
1:D:416:SER:HA	1:D:421:HIS:HB3	1.81	0.61
1:E:432:VAL:HG22	1:E:433:PRO:HD2	1.82	0.61
1:C:382:GLU:HB2	1:C:388:ILE:HB	1.82	0.61
1:E:331:HIS:CD2	1:E:333:ASP:H	2.19	0.61
1:D:178:LYS:HG2	1:D:227:GLU:OE2	2.01	0.61
1:C:420:ILE:HG13	1:C:420:ILE:O	2.00	0.61
1:D:198:GLN:HE22	1:D:250:GLN:NE2	1.98	0.61
1:A:284:GLU:HB3	1:A:343:LYS:CE	2.30	0.61
1:C:458:TRP:HZ3	1:C:471:MET:SD	2.23	0.61
1:C:443:LYS:HG3	1:C:447:GLU:OE1	2.01	0.61
1:B:377:ARG:NH1	3:B:11:PO4:O1	2.33	0.61
1:E:357:ARG:HB2	1:E:366:ASP:CB	2.30	0.60
1:D:216:PHE:HA	1:D:238:GLU:OE2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:466:VAL:O	1:C:470:ILE:HG13	2.01	0.60
1:D:310:ALA:HA	1:D:404:MET:CE	2.31	0.60
1:C:302:MET:HG3	1:C:411:ILE:HG22	1.82	0.60
1:C:377:ARG:HG3	1:C:436:PRO:HG2	1.83	0.60
1:B:432:VAL:HG11	1:B:436:PRO:HG3	1.84	0.60
1:A:381:PRO:HG3	1:A:445:VAL:CG1	2.31	0.60
1:C:425:GLN:HE21	1:C:425:GLN:HA	1.67	0.60
1:C:284:GLU:HB3	1:C:343:LYS:HZ2	1.65	0.59
1:D:459:GLN:NE2	1:D:465:ARG:HG3	2.17	0.59
1:A:464:LEU:O	1:A:464:LEU:HD13	2.01	0.59
1:D:331:HIS:HE1	1:D:350:ALA:O	1.85	0.59
1:C:287:SER:HA	1:C:339:ILE:O	2.02	0.59
1:D:294:ARG:HH11	1:D:294:ARG:HG2	1.68	0.59
1:E:331:HIS:HD2	1:E:333:ASP:N	1.99	0.59
1:A:331:HIS:HD2	1:A:333:ASP:H	1.49	0.59
1:A:413:ARG:HH12	1:A:422:GLU:HB3	1.67	0.59
1:C:459:GLN:HA	1:C:459:GLN:NE2	2.16	0.59
1:B:432:VAL:CG1	1:B:436:PRO:HG3	2.32	0.59
1:A:377:ARG:NH1	1:A:426:LEU:HD13	2.18	0.59
1:E:498:GLN:O	1:E:499:GLU:HG3	2.03	0.59
1:D:256:HIS:HD2	1:D:258:ASN:H	1.51	0.59
1:C:478:ASN:C	1:C:478:ASN:HD22	2.06	0.59
1:C:285:HIS:CB	1:C:341:VAL:HG13	2.33	0.58
1:D:204:THR:CG2	1:D:224:TRP:HE1	2.15	0.58
1:A:398:ARG:HD2	1:A:479:GLY:O	2.03	0.58
1:C:248:ILE:O	1:C:251:THR:HG23	2.03	0.58
1:A:443:LYS:HE2	1:A:448:GLN:HE22	1.68	0.58
1:D:294:ARG:HD3	1:D:295:TYR:CE2	2.38	0.58
1:E:322:GLY:HA3	1:E:324:GLN:HE22	1.68	0.58
1:E:389:ASN:HD21	1:E:391:LYS:HB3	1.68	0.58
1:C:215:ARG:CG	1:C:216:PHE:H	2.15	0.58
1:C:493:SER:O	1:C:497:GLN:HG3	2.02	0.58
1:D:178:LYS:HE2	1:D:227:GLU:OE2	2.04	0.58
1:C:442:ARG:HA	1:C:446:CYS:SG	2.43	0.58
1:C:487:ARG:NH1	1:C:490:LYS:HD3	2.18	0.58
1:A:413:ARG:HH11	1:A:413:ARG:HG2	1.68	0.58
1:A:221:ARG:HD2	1:A:282:TYR:OH	2.03	0.58
1:B:362:THR:O	1:B:364:THR:HG23	2.03	0.58
1:D:262:PHE:CD1	2:D:4:JZO:H1	2.38	0.58
1:D:377:ARG:HE	1:D:426:LEU:HB3	1.69	0.58
1:D:185:THR:C	1:D:187:SER:H	2.07	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:330:ALA:HB3	1:E:356:VAL:HG13	1.86	0.58
1:C:313:LEU:HD22	1:C:334:LEU:CD1	2.34	0.58
1:A:459:GLN:HB3	1:A:465:ARG:HD3	1.86	0.58
1:C:260:LEU:HD13	1:C:340:LEU:CD1	2.34	0.58
1:D:315:HIS:O	1:D:326:LYS:HE3	2.05	0.57
1:C:409:TRP:HA	1:C:471:MET:HE3	1.86	0.57
1:B:331:HIS:CD2	1:B:333:ASP:H	2.09	0.57
1:C:313:LEU:HD22	1:C:334:LEU:HD12	1.85	0.57
1:C:451:ARG:HE	1:C:475:TRP:HB3	1.69	0.57
1:D:487:ARG:NE	1:D:487:ARG:HA	2.19	0.57
1:B:365:ILE:HD11	1:B:367:ILE:HD13	1.86	0.57
1:C:183:ASP:O	1:C:187:SER:HB2	2.04	0.57
1:E:204:THR:CG2	1:E:224:TRP:NE1	2.65	0.57
1:A:364:THR:O	1:A:365:ILE:HG23	2.04	0.57
1:B:437:SER:OG	1:B:440:GLU:HG3	2.03	0.57
1:C:232:LYS:HE3	1:C:234:PHE:CZ	2.39	0.57
1:A:466:VAL:O	1:A:470:ILE:HG13	2.04	0.57
1:C:244:ARG:NH2	1:C:366:ASP:OD1	2.38	0.57
1:B:458:TRP:HZ3	1:B:471:MET:HE1	1.70	0.57
1:C:313:LEU:HB3	1:C:404:MET:HE1	1.87	0.57
1:B:215:ARG:HB3	1:B:215:ARG:NH1	2.19	0.57
1:D:368:ALA:HB2	1:E:178:LYS:HD3	1.87	0.56
1:A:463:ALA:HB2	1:A:495:LEU:HD11	1.86	0.56
1:C:331:HIS:CD2	1:C:333:ASP:H	2.23	0.56
1:D:215:ARG:HG2	1:D:215:ARG:HH11	1.69	0.56
1:A:297:VAL:HG22	1:A:298:THR:N	2.20	0.56
1:C:494:GLN:HA	1:C:497:GLN:NE2	2.20	0.56
1:D:342:LYS:HD3	1:D:346:THR:HG23	1.86	0.56
1:E:209:GLU:OE2	1:E:221:ARG:HD3	2.06	0.56
1:E:310:ALA:HA	1:E:404:MET:HE3	1.86	0.56
1:E:317:HIS:HB3	1:E:397:LYS:HE3	1.87	0.56
1:C:426:LEU:O	1:C:429:TYR:HB3	2.06	0.56
1:C:256:HIS:CD2	1:C:258:ASN:H	2.24	0.56
1:E:245:GLU:HB3	1:E:278:LEU:HD21	1.86	0.56
1:A:487:ARG:HE	1:A:491:THR:HG22	1.70	0.56
1:D:425:GLN:HB3	1:D:429:TYR:CD2	2.41	0.56
1:B:217:GLY:N	1:B:238:GLU:OE2	2.39	0.56
1:A:195:LEU:HD12	1:A:195:LEU:H	1.70	0.56
1:B:199:ARG:HH11	1:B:203:ARG:NH2	2.04	0.55
1:D:432:VAL:CG1	1:D:436:PRO:HG3	2.37	0.55
1:C:232:LYS:HE3	1:C:234:PHE:HZ	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:344:ASN:OD1	1:D:346:THR:HG22	2.07	0.55
1:E:435:ASP:N	1:E:436:PRO:HD3	2.21	0.55
1:D:309:THR:HG22	1:D:404:MET:HE2	1.87	0.55
1:E:389:ASN:ND2	1:E:391:LYS:HB3	2.21	0.55
1:E:214:GLY:O	1:E:215:ARG:C	2.44	0.55
1:E:256:HIS:CD2	1:E:257:GLU:N	2.74	0.55
1:C:313:LEU:HD11	1:C:317:HIS:NE2	2.21	0.55
1:C:283:HIS:ND1	3:C:10:PO4:O4	2.39	0.55
1:D:189:SER:O	1:D:191:SER:N	2.39	0.55
1:B:331:HIS:HD2	1:B:333:ASP:N	1.97	0.55
1:C:487:ARG:HH21	1:C:491:THR:HG22	1.71	0.55
1:D:272:THR:HG22	1:D:273:TRP:CD1	2.42	0.55
1:D:217:GLY:N	1:D:238:GLU:OE1	2.40	0.55
1:D:459:GLN:HE22	1:D:465:ARG:HG3	1.72	0.55
1:C:478:ASN:HD21	1:C:480:ALA:HB3	1.72	0.55
1:D:234:PHE:HA	1:D:238:GLU:OE1	2.06	0.55
1:A:177:LEU:N	1:A:227:GLU:OE2	2.40	0.55
1:A:301:GLY:HA2	1:A:304:LYS:HZ3	1.71	0.54
1:E:244:ARG:O	1:E:248:ILE:HG12	2.08	0.54
1:C:458:TRP:HE3	1:C:468:ALA:HB2	1.73	0.54
1:A:447:GLU:O	1:A:449:LYS:N	2.40	0.54
1:C:362:THR:HG22	1:C:364:THR:HG23	1.87	0.54
1:D:376:LYS:HD2	1:D:379:MET:HE1	1.89	0.54
1:C:258:ASN:O	1:C:348:CYS:HA	2.08	0.54
1:A:457:ARG:HH11	1:A:457:ARG:CB	2.20	0.54
1:C:438:VAL:O	1:C:442:ARG:HB2	2.07	0.54
1:B:434:SER:O	1:B:435:ASP:HB3	2.07	0.54
1:D:417:ILE:O	1:D:420:ILE:HG12	2.08	0.54
1:C:435:ASP:N	1:C:436:PRO:HD3	2.21	0.54
1:E:331:HIS:O	1:E:332:ARG:HB2	2.07	0.54
1:C:240:ARG:HH11	1:C:240:ARG:CB	2.20	0.54
1:C:417:ILE:HG12	1:C:461:CYS:SG	2.47	0.54
1:D:432:VAL:HG13	1:D:436:PRO:HG3	1.90	0.54
1:E:331:HIS:HE1	1:E:350:ALA:O	1.90	0.54
1:C:487:ARG:O	1:C:491:THR:HG23	2.08	0.54
1:C:293:ASN:HD22	1:C:424:TYR:HD2	1.55	0.54
1:B:197:VAL:O	1:B:201:ILE:HG12	2.08	0.54
1:E:473:GLU:HB3	1:E:483:LEU:HG	1.90	0.53
1:E:389:ASN:HD21	1:E:391:LYS:CB	2.21	0.53
1:A:251:THR:O	1:A:252:VAL:HG22	2.08	0.53
1:C:356:VAL:HG23	1:C:365:ILE:HG23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:417:ILE:HD11	1:D:457:ARG:HH11	1.74	0.53
1:B:409:TRP:HD1	1:B:471:MET:CE	2.22	0.53
1:D:372:ARG:NH1	1:D:438:VAL:HG11	2.24	0.53
1:E:372:ARG:NH1	1:E:383:VAL:O	2.42	0.53
1:B:246:ALA:O	1:B:250:GLN:HG3	2.08	0.53
1:A:486:LEU:O	1:A:489:LYS:HB3	2.09	0.53
1:B:331:HIS:HE1	1:B:350:ALA:O	1.92	0.53
1:E:184:MET:HB3	1:E:193:LEU:CD2	2.39	0.53
1:E:252:VAL:HG12	1:E:253:MET:N	2.21	0.53
1:B:333:ASP:HB2	1:B:354:LEU:HD12	1.91	0.53
1:A:498:GLN:CG	1:A:499:GLU:H	2.17	0.53
1:D:251:THR:O	1:D:252:VAL:CG2	2.54	0.53
1:D:294:ARG:HG2	1:D:294:ARG:O	2.08	0.53
1:B:413:ARG:NH1	1:B:422:GLU:HB3	2.24	0.53
1:C:232:LYS:HG2	1:C:234:PHE:CE1	2.43	0.53
1:D:331:HIS:CD2	1:D:333:ASP:H	2.22	0.53
1:C:372:ARG:HH12	1:C:438:VAL:HG11	1.73	0.52
1:C:256:HIS:HD2	1:C:258:ASN:HB2	1.74	0.52
1:C:483:LEU:H	1:C:483:LEU:HD12	1.73	0.52
1:B:430:ASP:O	1:B:431:LEU:HD23	2.08	0.52
1:C:288:LEU:HD12	1:C:292:LEU:HD13	1.92	0.52
1:E:198:GLN:HE22	1:E:250:GLN:NE2	2.07	0.52
1:D:259:ILE:CD1	1:D:316:LEU:HD13	2.39	0.52
1:C:403:ALA:O	1:C:407:VAL:HG23	2.09	0.52
1:C:408:PHE:O	1:C:411:ILE:HB	2.09	0.52
1:C:253:MET:HB3	1:C:326:LYS:CG	2.38	0.52
1:E:204:THR:HG22	1:E:224:TRP:CD1	2.45	0.52
1:A:459:GLN:O	1:A:465:ARG:NH1	2.43	0.52
1:A:214:GLY:O	1:A:215:ARG:C	2.48	0.52
1:C:472:ARG:C	1:C:474:CYS:H	2.12	0.52
1:C:244:ARG:HH12	1:C:366:ASP:HB3	1.74	0.52
1:D:469:LYS:HE2	1:D:473:GLU:OE2	2.10	0.52
1:A:487:ARG:HH21	1:A:491:THR:N	2.08	0.52
1:B:248:ILE:HD12	1:B:355:ALA:HB3	1.92	0.52
1:E:200:THR:O	1:E:204:THR:HB	2.09	0.52
1:D:389:ASN:ND2	1:D:389:ASN:C	2.59	0.52
1:C:317:HIS:HB3	1:C:397:LYS:HE2	1.92	0.52
1:C:278:LEU:HG	2:C:3:JZO:H1B	1.92	0.52
1:D:456:ASN:C	1:D:458:TRP:N	2.63	0.52
1:C:221:ARG:HD2	1:C:282:TYR:OH	2.09	0.52
1:E:377:ARG:NH1	3:E:3:PO4:O3	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:244:ARG:HH21	1:D:367:ILE:CG2	2.22	0.52
1:A:253:MET:HG2	1:A:324:GLN:O	2.10	0.52
1:A:296:THR:HG22	1:A:414:ARG:HH11	1.73	0.52
1:C:459:GLN:HE22	1:C:465:ARG:HG3	1.72	0.52
1:D:456:ASN:C	1:D:458:TRP:H	2.12	0.52
1:C:372:ARG:CZ	1:C:438:VAL:HG11	2.40	0.51
1:C:425:GLN:NE2	1:C:425:GLN:HA	2.25	0.51
1:A:488:ILE:O	1:A:492:LEU:HB2	2.11	0.51
1:A:216:PHE:HA	1:A:238:GLU:OE1	2.10	0.51
1:B:471:MET:O	1:B:474:CYS:HB2	2.10	0.51
1:A:260:LEU:HD23	4:A:504:HOH:O	2.11	0.51
1:C:209:GLU:OE1	1:C:221:ARG:NH1	2.43	0.51
1:E:417:ILE:HD11	1:E:464:LEU:HD21	1.91	0.51
1:A:462:GLU:O	1:A:466:VAL:HG23	2.09	0.51
1:C:479:GLY:HA2	1:C:482:ARG:CD	2.40	0.51
1:C:284:GLU:HB3	1:C:343:LYS:NZ	2.26	0.51
1:B:248:ILE:CD1	1:B:355:ALA:HB3	2.40	0.51
1:C:483:LEU:N	1:C:483:LEU:HD12	2.25	0.51
1:D:448:GLN:O	1:D:450:LEU:N	2.43	0.51
1:C:332:ARG:NH2	1:C:367:ILE:HG21	2.26	0.51
1:D:178:LYS:HE2	1:D:227:GLU:CD	2.31	0.51
1:A:195:LEU:CD1	1:A:195:LEU:H	2.24	0.51
1:A:344:ASN:OD1	1:A:346:THR:OG1	2.28	0.51
1:D:433:PRO:HG2	1:D:440:GLU:OE1	2.11	0.51
1:B:313:LEU:HD11	1:B:317:HIS:NE2	2.25	0.51
1:C:462:GLU:O	1:C:466:VAL:HG23	2.11	0.51
1:B:220:TRP:NE1	1:B:233:ILE:HD11	2.26	0.51
1:A:456:ASN:C	1:A:458:TRP:H	2.15	0.50
1:A:413:ARG:NH1	1:A:422:GLU:HB3	2.26	0.50
1:A:177:LEU:H	1:A:227:GLU:CD	2.15	0.50
1:A:407:VAL:O	1:A:411:ILE:HG13	2.11	0.50
1:C:181:ILE:HA	1:C:184:MET:CE	2.41	0.50
1:C:376:LYS:O	1:C:378:TYR:N	2.44	0.50
1:C:381:PRO:HD2	1:C:482:ARG:NH2	2.25	0.50
1:A:417:ILE:HG13	1:A:420:ILE:CD1	2.38	0.50
1:A:417:ILE:CG1	1:A:420:ILE:HD11	2.38	0.50
1:D:267:ASN:N	1:D:267:ASN:OD1	2.45	0.50
1:A:372:ARG:HD3	1:A:379:MET:HE1	1.93	0.50
1:B:253:MET:HE3	1:B:325:GLY:O	2.11	0.50
1:E:297:VAL:N	1:E:414:ARG:O	2.44	0.50
1:D:342:LYS:HD3	1:D:346:THR:CG2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:256:HIS:HB2	1:C:315:HIS:ND1	2.27	0.50
1:A:420:ILE:O	1:A:420:ILE:HG13	2.10	0.50
1:C:368:ALA:H	1:C:369:PRO:HD2	1.75	0.50
1:E:190:GLY:C	1:E:192:GLY:H	2.15	0.50
1:D:244:ARG:HH11	1:D:244:ARG:HG2	1.77	0.50
1:D:417:ILE:HD11	1:D:457:ARG:NH1	2.26	0.50
1:C:335:LYS:HG2	1:C:337:LYS:H	1.77	0.50
1:C:288:LEU:HB3	1:C:339:ILE:HB	1.93	0.50
1:B:377:ARG:HD3	1:B:427:PRO:HD2	1.92	0.50
1:A:431:LEU:HD13	1:A:444:VAL:CG1	2.41	0.50
1:D:205:ILE:CG2	1:D:206:VAL:N	2.75	0.50
1:C:468:ALA:HA	1:C:471:MET:SD	2.52	0.49
1:B:311:SER:HA	1:B:489:LYS:HG3	1.94	0.49
1:D:199:ARG:HD2	1:D:203:ARG:NH2	2.28	0.49
1:A:366:ASP:O	1:A:367:ILE:HB	2.10	0.49
1:A:328:ALA:HB1	1:A:393:PHE:CE2	2.47	0.49
1:D:443:LYS:O	1:D:447:GLU:HB2	2.12	0.49
1:C:198:GLN:HB3	1:C:264:ALA:HB1	1.93	0.49
1:A:470:ILE:HG23	1:A:483:LEU:CD1	2.42	0.49
1:A:215:ARG:HG2	1:A:215:ARG:HH11	1.78	0.49
1:C:409:TRP:HD1	1:C:471:MET:CE	2.25	0.49
1:C:406:LEU:H	1:C:406:LEU:HD22	1.78	0.49
1:B:385:ASP:HA	1:B:442:ARG:NH2	2.27	0.49
1:C:288:LEU:O	1:C:288:LEU:HD12	2.12	0.49
1:D:205:ILE:HG22	1:D:206:VAL:N	2.26	0.49
1:C:177:LEU:HB2	1:C:227:GLU:OE1	2.12	0.49
1:E:320:ILE:HD13	1:E:326:LYS:HG2	1.95	0.49
1:A:375:THR:O	1:A:379:MET:HG3	2.13	0.49
1:B:317:HIS:HB3	1:B:397:LYS:CE	2.36	0.49
1:C:448:GLN:HB2	1:C:450:LEU:HG	1.94	0.49
1:C:476:TYR:O	1:C:478:ASN:N	2.45	0.49
1:D:381:PRO:HG3	1:D:445:VAL:CG1	2.42	0.49
1:A:304:LYS:HB2	1:A:304:LYS:HZ3	1.77	0.49
1:B:433:PRO:HG2	1:B:440:GLU:OE2	2.11	0.49
1:D:368:ALA:HB2	1:E:178:LYS:HG2	1.94	0.49
1:D:459:GLN:O	1:D:465:ARG:NH1	2.46	0.49
1:B:199:ARG:HD3	1:B:203:ARG:CZ	2.42	0.49
1:B:195:LEU:H	1:B:195:LEU:CD1	2.25	0.49
1:C:402:TYR:CE1	1:C:406:LEU:HD21	2.48	0.49
1:C:260:LEU:HD13	1:C:340:LEU:HD13	1.94	0.49
1:B:337:LYS:HD2	3:B:12:PO4:O2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:253:MET:HG3	1:E:326:LYS:H	1.76	0.49
1:D:426:LEU:O	1:D:429:TYR:HB3	2.13	0.49
1:D:448:GLN:HB2	1:D:450:LEU:HD12	1.94	0.49
1:E:385:ASP:HA	1:E:442:ARG:HD2	1.95	0.49
1:C:417:ILE:H	1:C:420:ILE:CG1	2.26	0.49
1:C:406:LEU:N	1:C:406:LEU:HD22	2.28	0.49
1:E:432:VAL:HG22	1:E:433:PRO:CD	2.43	0.49
1:C:258:ASN:OD1	1:C:308:SER:HB2	2.13	0.49
1:D:259:ILE:HD13	1:D:316:LEU:HD13	1.94	0.49
1:E:242:TRP:CD1	1:E:278:LEU:HD13	2.47	0.48
1:A:251:THR:OG1	1:A:251:THR:O	2.30	0.48
1:D:441:MET:O	1:D:442:ARG:C	2.51	0.48
1:C:197:VAL:O	1:C:201:ILE:HG13	2.12	0.48
1:C:334:LEU:HD23	1:C:335:LYS:H	1.78	0.48
1:D:417:ILE:HG13	1:D:420:ILE:CG1	2.34	0.48
1:B:282:TYR:HE2	1:B:284:GLU:HG2	1.78	0.48
1:B:287:SER:HA	1:B:339:ILE:O	2.13	0.48
1:E:237:ARG:HG2	1:E:237:ARG:O	2.13	0.48
1:B:372:ARG:NH2	1:B:438:VAL:HG11	2.29	0.48
1:B:392:HIS:O	1:B:395:SER:HB3	2.12	0.48
1:C:303:ILE:HG21	1:C:496:SER:HB2	1.95	0.48
1:C:199:ARG:HD2	1:C:203:ARG:NE	2.29	0.48
1:C:320:ILE:CG2	1:C:321:VAL:N	2.76	0.48
1:A:447:GLU:C	1:A:449:LYS:H	2.17	0.48
1:C:413:ARG:HG3	1:C:422:GLU:HB2	1.95	0.48
1:A:242:TRP:CD1	1:A:276:LEU:HB3	2.48	0.48
1:C:302:MET:CE	1:C:467:MET:HG3	2.44	0.48
1:C:253:MET:HE2	1:C:325:GLY:HA2	1.96	0.48
1:A:328:ALA:HB1	1:A:393:PHE:HE2	1.77	0.48
1:C:307:LEU:HD22	1:C:493:SER:HA	1.95	0.48
1:A:195:LEU:N	1:A:195:LEU:HD12	2.28	0.48
1:C:414:ARG:HH11	1:C:414:ARG:CA	2.27	0.48
1:B:258:ASN:O	1:B:348:CYS:HA	2.13	0.48
1:B:186:THR:O	1:B:186:THR:HG22	2.13	0.48
1:E:447:GLU:O	1:E:449:LYS:HG3	2.13	0.48
1:C:406:LEU:CD2	1:C:406:LEU:H	2.27	0.48
1:B:376:LYS:HD2	1:B:379:MET:HE3	1.95	0.48
1:B:191:SER:HB2	1:B:250:GLN:HA	1.96	0.48
1:B:253:MET:CE	1:B:325:GLY:N	2.77	0.48
1:D:459:GLN:HA	1:D:459:GLN:NE2	2.29	0.48
1:C:183:ASP:O	1:C:187:SER:CB	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:215:ARG:HG3	1:E:215:ARG:NH1	2.29	0.48
1:C:382:GLU:H	1:C:382:GLU:CD	2.16	0.48
1:A:459:GLN:HA	1:A:465:ARG:CG	2.43	0.48
1:D:454:ILE:HG23	1:D:458:TRP:CE3	2.49	0.48
1:D:342:LYS:HE3	1:D:348:CYS:HB3	1.96	0.47
1:D:431:LEU:CD1	1:D:450:LEU:HD13	2.44	0.47
1:A:315:HIS:HE1	1:A:326:LYS:HD2	1.79	0.47
1:D:244:ARG:HH21	1:D:367:ILE:HG22	1.78	0.47
1:A:393:PHE:O	1:A:395:SER:N	2.47	0.47
1:C:211:ILE:HD12	2:C:3:JZO:C24	2.44	0.47
1:C:256:HIS:CD2	1:C:258:ASN:HB2	2.49	0.47
1:A:252:VAL:HG23	1:A:253:MET:N	2.29	0.47
1:A:232:LYS:HE3	1:A:234:PHE:CZ	2.49	0.47
1:B:317:HIS:CB	1:B:397:LYS:HE3	2.36	0.47
1:B:376:LYS:HD2	1:B:379:MET:CE	2.44	0.47
1:C:365:ILE:CG2	1:C:366:ASP:N	2.77	0.47
1:D:216:PHE:CA	1:D:238:GLU:OE2	2.62	0.47
1:E:181:ILE:HA	1:E:184:MET:CE	2.45	0.47
1:E:310:ALA:CA	1:E:404:MET:HE3	2.44	0.47
1:E:285:HIS:HB2	1:E:341:VAL:HG22	1.97	0.47
1:C:464:LEU:H	1:C:464:LEU:HD22	1.79	0.47
1:C:452:PRO:HD2	1:C:475:TRP:CZ3	2.49	0.47
1:C:415:CYS:SG	1:C:416:SER:N	2.88	0.47
1:E:181:ILE:O	1:E:184:MET:HG2	2.15	0.47
1:C:343:LYS:C	1:C:345:GLY:H	2.18	0.47
1:A:331:HIS:HD2	1:A:333:ASP:N	2.12	0.47
1:A:459:GLN:C	1:A:465:ARG:HH11	2.18	0.47
1:A:434:SER:O	1:A:435:ASP:HB3	2.14	0.47
1:B:187:SER:O	1:B:189:SER:N	2.47	0.47
1:A:248:ILE:CD1	1:A:355:ALA:HB3	2.44	0.47
1:E:253:MET:CE	1:E:320:ILE:HG21	2.45	0.47
1:A:358:HIS:HB2	1:A:393:PHE:CD1	2.50	0.47
1:D:424:TYR:OH	1:D:426:LEU:HD23	2.15	0.47
1:E:310:ALA:HB2	1:E:404:MET:HE1	1.97	0.47
1:D:297:VAL:HG22	1:D:298:THR:O	2.15	0.47
1:C:365:ILE:HG22	1:C:366:ASP:N	2.30	0.47
1:C:381:PRO:HD3	1:C:402:TYR:CE2	2.50	0.47
1:B:215:ARG:HB3	1:B:215:ARG:CZ	2.44	0.47
1:A:294:ARG:HH11	1:A:294:ARG:HG2	1.78	0.47
1:D:244:ARG:NH1	1:D:244:ARG:HG2	2.30	0.47
1:C:189:SER:C	1:C:191:SER:H	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:LYS:HG3	1:C:275:GLN:HB2	1.95	0.47
1:E:460:SER:O	1:E:465:ARG:NH1	2.48	0.47
1:E:199:ARG:O	1:E:203:ARG:HG3	2.14	0.46
1:C:287:SER:C	1:C:289:PHE:N	2.69	0.46
1:A:406:LEU:HD22	1:A:427:PRO:HB3	1.97	0.46
1:B:303:ILE:CD1	1:B:499:GLU:HG3	2.45	0.46
1:A:409:TRP:HA	1:A:471:MET:HE1	1.97	0.46
3:E:2:PO4:O1	3:E:3:PO4:O1	2.34	0.46
1:E:232:LYS:HG2	1:E:234:PHE:CE1	2.50	0.46
1:C:457:ARG:HG3	1:C:458:TRP:HD1	1.80	0.46
1:C:320:ILE:CG2	1:C:321:VAL:H	2.24	0.46
1:A:450:LEU:O	1:A:451:ARG:HD2	2.14	0.46
1:D:403:ALA:O	1:D:407:VAL:HG23	2.16	0.46
1:D:460:SER:OG	1:D:461:CYS:N	2.49	0.46
1:E:258:ASN:HD22	1:E:311:SER:HB2	1.79	0.46
1:C:244:ARG:NH1	1:C:366:ASP:HB3	2.31	0.46
1:E:432:VAL:CG2	1:E:433:PRO:HD2	2.46	0.46
1:A:459:GLN:OE1	1:A:465:ARG:HG2	2.16	0.46
1:B:251:THR:HG21	1:B:327:PRO:HD2	1.97	0.46
1:E:294:ARG:HG2	1:E:294:ARG:HH11	1.80	0.46
1:E:287:SER:HA	1:E:339:ILE:O	2.16	0.46
1:D:389:ASN:HD21	1:D:391:LYS:CB	2.23	0.46
3:D:15:PO4:O1	3:D:14:PO4:O4	2.34	0.46
1:A:412:ALA:C	1:A:414:ARG:H	2.18	0.46
1:A:184:MET:C	1:A:186:THR:H	2.18	0.46
1:A:199:ARG:O	1:A:203:ARG:HG2	2.16	0.46
1:C:302:MET:HE1	1:C:467:MET:HG3	1.97	0.46
1:B:432:VAL:HG13	1:B:433:PRO:HD2	1.97	0.46
1:B:449:LYS:HB2	1:B:449:LYS:NZ	2.31	0.46
1:D:429:TYR:CZ	1:D:430:ASP:OD2	2.69	0.46
1:B:195:LEU:N	1:B:195:LEU:HD12	2.31	0.46
1:B:334:LEU:O	1:B:335:LYS:HB3	2.16	0.46
1:D:185:THR:O	1:D:187:SER:N	2.49	0.46
1:C:409:TRP:CD1	1:C:471:MET:HE3	2.51	0.46
1:C:428:TYR:O	1:C:432:VAL:HG12	2.16	0.46
1:A:365:ILE:O	1:A:367:ILE:N	2.49	0.46
1:C:478:ASN:C	1:C:478:ASN:ND2	2.69	0.46
1:D:431:LEU:HD13	1:D:450:LEU:HD13	1.98	0.46
1:A:417:ILE:O	1:A:420:ILE:HG12	2.17	0.46
1:B:365:ILE:O	1:B:365:ILE:HG13	2.13	0.46
1:D:431:LEU:HD11	1:D:450:LEU:HD22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:443:LYS:HG2	1:E:448:GLN:HE21	1.80	0.46
1:C:213:LYS:HG2	1:C:218:GLU:HG3	1.97	0.46
1:D:295:TYR:O	1:D:414:ARG:NH1	2.49	0.45
1:E:454:ILE:HG23	1:E:458:TRP:CE3	2.51	0.45
1:C:406:LEU:O	1:C:410:GLU:HG3	2.16	0.45
1:A:455:PRO:HB2	1:A:458:TRP:CD1	2.51	0.45
1:A:413:ARG:NH1	1:A:423:ASP:O	2.49	0.45
1:E:385:ASP:C	1:E:385:ASP:OD2	2.54	0.45
1:A:320:ILE:HB	1:A:326:LYS:H	1.80	0.45
1:E:237:ARG:O	1:E:237:ARG:CG	2.64	0.45
1:A:409:TRP:HA	1:A:471:MET:CE	2.46	0.45
1:E:342:LYS:HG2	1:E:346:THR:O	2.16	0.45
1:C:302:MET:HG3	1:C:411:ILE:CG2	2.45	0.45
1:C:324:GLN:HG3	1:C:325:GLY:N	2.32	0.45
1:D:435:ASP:N	1:D:436:PRO:HD3	2.31	0.45
1:E:494:GLN:O	1:E:497:GLN:HB3	2.16	0.45
1:E:285:HIS:CB	1:E:341:VAL:HG22	2.47	0.45
1:E:413:ARG:NH1	1:E:423:ASP:O	2.48	0.45
1:D:443:LYS:HA	1:D:447:GLU:HG3	1.98	0.45
1:D:310:ALA:HA	1:D:404:MET:HE2	1.98	0.45
1:A:426:LEU:O	1:A:429:TYR:HB3	2.17	0.45
1:B:472:ARG:C	1:B:474:CYS:H	2.20	0.45
1:A:432:VAL:HG21	1:A:436:PRO:HB3	1.98	0.45
1:B:479:GLY:HA2	1:B:482:ARG:HD2	1.99	0.45
1:C:418:GLY:C	1:C:420:ILE:H	2.20	0.45
1:B:200:THR:O	1:B:204:THR:HB	2.17	0.45
1:C:278:LEU:HD12	1:C:278:LEU:HA	1.81	0.45
1:A:294:ARG:NH1	1:A:294:ARG:HG2	2.32	0.45
1:B:492:LEU:HD12	1:B:492:LEU:HA	1.65	0.45
1:C:310:ALA:HA	1:C:404:MET:CE	2.46	0.45
1:C:407:VAL:O	1:C:408:PHE:C	2.54	0.45
1:B:342:LYS:HD3	1:B:346:THR:HG22	1.99	0.45
1:E:461:CYS:HB3	1:E:464:LEU:HD23	1.98	0.45
1:A:331:HIS:CD2	1:A:333:ASP:H	2.33	0.45
1:C:340:LEU:O	1:C:347:CYS:HA	2.17	0.45
1:E:459:GLN:NE2	1:E:459:GLN:HA	2.32	0.45
1:B:412:ALA:O	1:B:414:ARG:N	2.50	0.45
1:A:251:THR:HG21	1:A:357:ARG:HD3	1.98	0.45
1:D:372:ARG:HH11	1:D:438:VAL:HG21	1.81	0.45
1:A:215:ARG:HH21	1:A:354:LEU:HD11	1.82	0.45
1:C:332:ARG:HG3	1:C:356:VAL:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:244:ARG:HH21	1:E:248:ILE:HD11	1.82	0.45
1:A:458:TRP:CG	1:A:464:LEU:HD11	2.52	0.45
1:E:299:VAL:O	1:E:303:ILE:HG13	2.16	0.45
1:B:404:MET:O	1:B:407:VAL:HB	2.17	0.45
1:D:469:LYS:HD2	1:D:472:ARG:HH21	1.83	0.44
1:D:413:ARG:NH1	1:D:423:ASP:O	2.50	0.44
1:B:432:VAL:HG13	1:B:433:PRO:CD	2.47	0.44
1:B:431:LEU:HD13	1:B:450:LEU:HD13	1.99	0.44
1:B:204:THR:CG2	1:B:224:TRP:NE1	2.78	0.44
1:D:310:ALA:HA	1:D:404:MET:HE1	2.00	0.44
1:E:198:GLN:HE22	1:E:250:GLN:HE22	1.64	0.44
1:A:292:LEU:HD21	1:A:411:ILE:HA	1.98	0.44
1:A:294:ARG:O	1:A:295:TYR:CG	2.70	0.44
1:C:268:LYS:CG	1:C:275:GLN:HB2	2.46	0.44
1:D:329:ILE:HA	1:D:356:VAL:O	2.17	0.44
1:C:486:LEU:O	1:C:489:LYS:HB3	2.18	0.44
1:A:430:ASP:OD1	1:A:431:LEU:HG	2.18	0.44
1:A:432:VAL:CG2	1:A:433:PRO:HD2	2.47	0.44
1:E:412:ALA:C	1:E:414:ARG:H	2.21	0.44
1:B:377:ARG:HH12	3:B:11:PO4:P	2.40	0.44
1:E:310:ALA:HA	1:E:404:MET:CE	2.47	0.44
1:A:435:ASP:N	1:A:436:PRO:HD3	2.32	0.44
1:E:358:HIS:HB2	1:E:393:PHE:CD1	2.52	0.44
1:A:484:THR:O	1:A:488:ILE:HG13	2.17	0.44
1:C:389:ASN:HD21	1:C:391:LYS:HB3	1.81	0.44
1:D:294:ARG:HD3	1:D:295:TYR:CZ	2.52	0.44
1:A:393:PHE:O	1:A:394:GLU:C	2.56	0.44
1:B:412:ALA:C	1:B:414:ARG:N	2.71	0.44
1:B:487:ARG:O	1:B:491:THR:HG23	2.18	0.44
1:C:342:LYS:HB2	1:C:344:ASN:OD1	2.17	0.44
1:E:237:ARG:NH1	1:E:238:GLU:OE2	2.51	0.44
1:B:204:THR:HG22	1:B:224:TRP:HE1	1.81	0.44
1:B:416:SER:HA	1:B:421:HIS:HB3	1.98	0.44
1:B:178:LYS:HD3	1:B:227:GLU:OE2	2.17	0.44
1:C:319:GLU:OE2	1:C:360:SER:HB3	2.17	0.44
1:B:376:LYS:HA	1:B:379:MET:HE2	1.95	0.44
1:D:217:GLY:CA	1:D:238:GLU:OE1	2.66	0.44
1:A:298:THR:CG2	1:A:299:VAL:N	2.80	0.44
1:C:405:GLY:HA3	1:C:475:TRP:HE1	1.83	0.44
1:C:319:GLU:HG2	1:C:320:ILE:N	2.31	0.44
1:E:489:LYS:O	1:E:493:SER:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:409:TRP:HD1	1:C:471:MET:HE3	1.82	0.43
1:C:483:LEU:CD1	1:C:488:ILE:HD11	2.46	0.43
1:B:432:VAL:HG11	1:B:436:PRO:CG	2.48	0.43
1:C:368:ALA:N	1:C:369:PRO:CD	2.80	0.43
1:E:184:MET:HG3	1:E:185:THR:N	2.33	0.43
1:A:323:THR:OG1	1:A:324:GLN:N	2.51	0.43
1:E:211:ILE:HD12	2:E:5:JZO:C24	2.49	0.43
1:B:385:ASP:O	1:B:387:SER:N	2.51	0.43
1:D:232:LYS:HG2	1:D:234:PHE:CE1	2.54	0.43
1:A:331:HIS:HE1	1:A:350:ALA:O	2.01	0.43
1:D:424:TYR:O	1:D:425:GLN:NE2	2.51	0.43
1:A:412:ALA:C	1:A:414:ARG:N	2.70	0.43
1:C:417:ILE:H	1:C:420:ILE:HG13	1.83	0.43
1:A:381:PRO:HG3	1:A:445:VAL:HG12	1.99	0.43
1:D:309:THR:HG22	1:D:404:MET:CE	2.47	0.43
1:C:425:GLN:CA	1:C:425:GLN:HE21	2.28	0.43
1:A:425:GLN:HB3	1:A:429:TYR:CD2	2.52	0.43
1:C:476:TYR:C	1:C:478:ASN:N	2.72	0.43
1:C:478:ASN:ND2	1:C:480:ALA:H	2.16	0.43
1:C:422:GLU:OE1	1:C:422:GLU:N	2.51	0.43
1:C:406:LEU:HB3	1:C:427:PRO:HG2	1.99	0.43
1:C:334:LEU:HD23	1:C:335:LYS:N	2.34	0.43
1:C:313:LEU:N	1:C:349:ILE:HD11	2.34	0.43
1:C:496:SER:C	1:C:498:GLN:H	2.21	0.43
1:B:209:GLU:OE2	1:B:221:ARG:NH1	2.51	0.43
1:C:297:VAL:HG13	1:C:298:THR:N	2.32	0.43
1:C:199:ARG:O	1:C:203:ARG:HG3	2.18	0.43
1:A:358:HIS:HB2	1:A:393:PHE:CE1	2.53	0.43
1:C:476:TYR:O	1:C:477:ALA:C	2.56	0.43
1:C:217:GLY:HA3	1:C:234:PHE:HA	2.01	0.43
1:C:262:PHE:CD1	2:C:3:JZO:H1	2.54	0.43
1:E:461:CYS:SG	1:E:464:LEU:HD23	2.59	0.43
1:B:385:ASP:HB2	1:B:442:ARG:HH21	1.83	0.43
1:E:306:ALA:HB1	1:E:492:LEU:HD21	2.00	0.43
1:B:269:ASP:HB3	1:B:270:ASN:H	1.63	0.43
1:E:297:VAL:O	1:E:415:CYS:HA	2.19	0.43
1:D:234:PHE:CE1	1:D:278:LEU:HD22	2.53	0.43
1:C:234:PHE:CE1	1:C:278:LEU:HD22	2.54	0.43
1:D:438:VAL:HG12	1:D:439:GLU:N	2.33	0.43
1:E:492:LEU:HD12	1:E:492:LEU:HA	1.66	0.43
1:B:300:GLU:HG3	1:B:501:ILE:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:GLU:HG3	1:A:500:GLY:H	1.84	0.43
1:D:331:HIS:HD2	1:D:333:ASP:N	2.12	0.43
1:C:181:ILE:HA	1:C:184:MET:HE2	2.00	0.43
1:E:416:SER:HA	1:E:421:HIS:HB3	2.00	0.43
1:D:371:HIS:N	1:D:371:HIS:ND1	2.66	0.43
1:B:319:GLU:HB2	1:B:328:ALA:HB2	2.01	0.43
1:C:414:ARG:HH11	1:C:414:ARG:HA	1.84	0.43
1:C:484:THR:O	1:C:488:ILE:HG13	2.19	0.43
1:B:495:LEU:O	1:B:499:GLU:HG2	2.18	0.43
1:C:488:ILE:HG22	1:C:488:ILE:O	2.18	0.42
1:C:372:ARG:NH2	1:C:438:VAL:HG11	2.34	0.42
1:B:343:LYS:HG3	3:B:6:PO4:P	2.59	0.42
1:E:254:LEU:HA	1:E:254:LEU:HD12	1.80	0.42
1:C:432:VAL:HA	1:C:433:PRO:HD3	1.81	0.42
1:C:483:LEU:HD13	1:C:488:ILE:CD1	2.48	0.42
1:A:215:ARG:NH2	1:A:354:LEU:HD11	2.33	0.42
1:A:409:TRP:CE2	1:A:452:PRO:HB3	2.54	0.42
1:B:389:ASN:HD21	1:B:391:LYS:HB2	1.84	0.42
1:D:181:ILE:HG12	1:D:184:MET:HE2	2.01	0.42
1:C:297:VAL:CG1	1:C:415:CYS:HA	2.49	0.42
1:E:199:ARG:HD2	1:E:203:ARG:NE	2.34	0.42
1:D:262:PHE:HD1	2:D:4:JZO:C1	2.31	0.42
1:E:180:LEU:HD13	1:E:201:ILE:HD11	2.02	0.42
1:D:429:TYR:CE1	1:D:430:ASP:HB3	2.53	0.42
1:A:315:HIS:CE1	1:A:326:LYS:CD	3.02	0.42
1:B:412:ALA:C	1:B:414:ARG:H	2.23	0.42
1:E:479:GLY:HA2	1:E:482:ARG:CZ	2.49	0.42
1:D:197:VAL:O	1:D:201:ILE:HG13	2.19	0.42
1:C:492:LEU:HD12	1:C:495:LEU:HD23	2.01	0.42
1:C:237:ARG:CD	1:C:238:GLU:OE2	2.66	0.42
1:D:234:PHE:HB3	1:D:238:GLU:HG3	2.01	0.42
1:A:335:LYS:O	1:A:339:ILE:HG13	2.19	0.42
1:C:298:THR:O	1:C:301:GLY:N	2.52	0.42
1:C:402:TYR:C	1:C:402:TYR:CD1	2.93	0.42
1:C:410:GLU:O	1:C:414:ARG:HG2	2.19	0.42
1:A:456:ASN:O	1:A:458:TRP:N	2.52	0.42
1:A:447:GLU:C	1:A:449:LYS:N	2.73	0.42
1:E:377:ARG:NH1	3:E:3:PO4:O4	2.50	0.42
1:B:388:ILE:HG13	1:B:395:SER:OG	2.19	0.42
1:B:319:GLU:C	1:B:320:ILE:HG13	2.39	0.42
1:A:198:GLN:HB3	1:A:264:ALA:HB1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:464:LEU:CD2	1:C:464:LEU:H	2.32	0.42
1:C:367:ILE:O	1:C:367:ILE:HG22	2.19	0.42
1:B:342:LYS:HB2	1:B:346:THR:HG22	2.02	0.42
1:D:443:LYS:HA	1:D:447:GLU:HG2	1.99	0.42
1:E:389:ASN:ND2	1:E:391:LYS:CB	2.82	0.42
1:E:310:ALA:N	1:E:404:MET:HE3	2.34	0.42
1:D:444:VAL:O	1:D:450:LEU:HB2	2.20	0.42
1:A:184:MET:O	1:A:186:THR:N	2.52	0.42
1:D:208:GLN:C	1:D:209:GLU:HG3	2.40	0.42
1:B:478:ASN:OD1	1:B:478:ASN:C	2.58	0.42
1:C:418:GLY:C	1:C:420:ILE:N	2.73	0.42
1:C:379:MET:CE	1:C:383:VAL:HG11	2.49	0.42
1:D:473:GLU:O	1:D:482:ARG:HA	2.19	0.42
1:E:270:ASN:O	1:E:271:GLY:C	2.57	0.42
1:C:216:PHE:HA	1:C:238:GLU:HG3	2.02	0.42
1:C:470:ILE:HG21	1:C:488:ILE:HG23	2.01	0.42
1:C:259:ILE:O	1:C:260:LEU:C	2.57	0.42
1:B:409:TRP:CD1	1:B:471:MET:CE	3.03	0.42
1:D:364:THR:C	1:D:365:ILE:HD12	2.39	0.42
1:C:215:ARG:HH11	1:C:215:ARG:CG	2.32	0.42
1:A:454:ILE:O	1:A:455:PRO:C	2.58	0.42
1:C:307:LEU:HD12	1:C:307:LEU:O	2.19	0.42
1:C:287:SER:C	1:C:289:PHE:H	2.23	0.42
1:C:334:LEU:HD21	1:C:339:ILE:HD11	2.02	0.42
1:E:180:LEU:O	1:E:181:ILE:C	2.58	0.42
1:A:315:HIS:ND1	1:A:315:HIS:O	2.52	0.42
1:B:294:ARG:O	1:B:294:ARG:HD3	2.20	0.42
1:A:493:SER:O	1:A:496:SER:HB3	2.19	0.42
1:B:205:ILE:CG2	1:B:206:VAL:N	2.83	0.42
1:A:317:HIS:HE1	1:A:400:ASP:HB2	1.84	0.42
1:C:177:LEU:HA	1:C:177:LEU:HD23	1.85	0.42
1:A:199:ARG:HD2	1:A:266:ASP:OD2	2.20	0.42
1:C:253:MET:HG3	1:C:253:MET:O	2.20	0.41
1:B:331:HIS:O	1:B:332:ARG:HB2	2.20	0.41
1:C:333:ASP:HB2	1:C:354:LEU:HD12	2.02	0.41
1:C:486:LEU:HD13	1:C:486:LEU:O	2.20	0.41
1:A:257:GLU:O	1:A:257:GLU:HG2	2.19	0.41
1:C:414:ARG:HD2	1:C:414:ARG:HA	1.78	0.41
1:D:391:LYS:HG2	1:D:391:LYS:O	2.20	0.41
1:C:254:LEU:HD12	1:C:254:LEU:HA	1.88	0.41
1:A:413:ARG:HH11	1:A:413:ARG:CG	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:TYR:OH	1:A:426:LEU:HD23	2.21	0.41
1:A:308:SER:HB3	1:A:346:THR:HG22	2.02	0.41
1:B:294:ARG:HD2	1:B:295:TYR:CZ	2.54	0.41
1:B:490:LYS:HB2	1:B:490:LYS:HE3	1.86	0.41
1:A:310:ALA:HA	1:A:404:MET:HE1	2.01	0.41
1:C:443:LYS:O	1:C:448:GLN:NE2	2.54	0.41
1:A:297:VAL:CG2	1:A:298:THR:N	2.83	0.41
1:D:344:ASN:OD1	1:D:346:THR:CG2	2.68	0.41
1:B:195:LEU:H	1:B:195:LEU:HD12	1.85	0.41
1:B:393:PHE:O	1:B:395:SER:N	2.53	0.41
1:E:455:PRO:HD2	1:E:458:TRP:CE2	2.55	0.41
1:B:234:PHE:CE1	1:B:278:LEU:HD22	2.55	0.41
1:B:459:GLN:O	1:B:465:ARG:HD3	2.20	0.41
1:C:471:MET:HE1	1:C:475:TRP:HH2	1.84	0.41
1:D:278:LEU:HD12	1:D:278:LEU:HA	1.91	0.41
1:E:201:ILE:O	1:E:205:ILE:HG13	2.21	0.41
1:D:214:GLY:O	1:D:215:ARG:C	2.59	0.41
1:B:193:LEU:HB3	1:B:194:PRO:CD	2.50	0.41
1:A:429:TYR:CG	1:A:430:ASP:N	2.88	0.41
1:D:185:THR:C	1:D:187:SER:N	2.73	0.41
1:B:426:LEU:O	1:B:429:TYR:HB3	2.20	0.41
1:C:416:SER:C	1:C:417:ILE:HD12	2.41	0.41
1:E:253:MET:CE	1:E:325:GLY:HA2	2.50	0.41
1:D:180:LEU:HD13	1:D:201:ILE:HD11	2.03	0.41
1:C:208:GLN:NE2	1:C:223:LYS:HD2	2.35	0.41
1:B:330:ALA:HB3	1:B:356:VAL:HG22	2.02	0.41
1:E:194:PRO:O	1:E:197:VAL:N	2.54	0.41
1:C:240:ARG:CG	1:C:240:ARG:HH11	2.33	0.41
1:E:185:THR:O	1:E:185:THR:HG22	2.21	0.41
1:D:455:PRO:HD2	1:D:458:TRP:CE3	2.56	0.41
1:E:337:LYS:NZ	3:E:2:PO4:O1	2.49	0.41
1:D:498:GLN:O	1:D:499:GLU:CG	2.69	0.41
1:A:285:HIS:HB3	1:A:341:VAL:HG22	2.03	0.41
1:A:494:GLN:O	1:A:497:GLN:N	2.50	0.41
1:A:244:ARG:HD2	1:A:244:ARG:HA	1.85	0.41
1:D:462:GLU:O	1:D:463:ALA:C	2.59	0.41
1:D:331:HIS:CE1	1:D:350:ALA:O	2.69	0.41
1:A:317:HIS:NE2	1:A:400:ASP:OD2	2.53	0.41
1:C:458:TRP:HB3	1:C:464:LEU:HB3	2.02	0.41
1:C:330:ALA:HB3	1:C:356:VAL:HG13	2.02	0.41
1:C:398:ARG:HD3	1:C:479:GLY:C	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:LEU:CD1	1:B:450:LEU:HD13	2.51	0.41
1:C:310:ALA:HA	1:C:404:MET:HE1	2.02	0.41
1:B:455:PRO:HD2	1:B:458:TRP:CD2	2.56	0.41
1:D:215:ARG:HG2	1:D:215:ARG:NH1	2.35	0.41
1:E:215:ARG:HG3	1:E:215:ARG:HH11	1.84	0.41
1:B:393:PHE:C	1:B:395:SER:N	2.74	0.41
1:C:496:SER:C	1:C:498:GLN:N	2.75	0.41
1:A:256:HIS:CD2	1:A:258:ASN:H	2.38	0.41
1:A:258:ASN:OD1	1:A:311:SER:HB2	2.21	0.41
1:D:305:LEU:HD23	1:D:345:GLY:O	2.21	0.41
1:B:417:ILE:O	1:B:420:ILE:HG12	2.20	0.41
1:A:328:ALA:HB3	1:A:358:HIS:HB3	2.03	0.41
1:C:331:HIS:CD2	1:C:333:ASP:C	2.94	0.41
1:E:384:LEU:O	1:E:442:ARG:HG3	2.21	0.41
1:A:476:TYR:C	1:A:478:ASN:H	2.24	0.41
1:C:216:PHE:HB3	1:C:238:GLU:HB3	2.03	0.40
1:C:478:ASN:ND2	1:C:480:ALA:HB3	2.37	0.40
1:E:459:GLN:NE2	1:E:465:ARG:HD2	2.35	0.40
1:E:196:LEU:HA	1:E:196:LEU:HD12	1.93	0.40
1:D:492:LEU:HA	1:D:492:LEU:HD12	1.76	0.40
1:A:278:LEU:HA	1:A:278:LEU:HD23	1.95	0.40
1:E:437:SER:OG	1:E:440:GLU:HG3	2.22	0.40
1:C:417:ILE:N	1:C:417:ILE:HD12	2.36	0.40
1:D:490:LYS:HE3	1:D:490:LYS:HB2	1.84	0.40
1:E:181:ILE:HA	1:E:184:MET:HE2	2.04	0.40
1:D:453:ASN:O	1:D:455:PRO:HD3	2.20	0.40
1:A:283:HIS:H	2:A:1:JZO:C23	2.35	0.40
1:D:235:SER:O	1:D:236:SER:C	2.60	0.40
1:C:286:GLY:O	1:C:340:LEU:HA	2.22	0.40
1:A:428:TYR:CE2	1:A:452:PRO:HD3	2.56	0.40
1:B:234:PHE:CD1	1:B:234:PHE:N	2.89	0.40
1:C:376:LYS:C	1:C:378:TYR:N	2.73	0.40
1:E:497:GLN:C	1:E:499:GLU:H	2.24	0.40
1:C:181:ILE:HA	1:C:184:MET:HE3	2.03	0.40
1:D:297:VAL:CG2	1:D:301:GLY:HA3	2.51	0.40
1:B:424:TYR:C	1:B:424:TYR:CD2	2.95	0.40
1:A:453:ASN:O	1:A:455:PRO:HD3	2.21	0.40
1:A:398:ARG:HG3	1:A:398:ARG:NH1	2.36	0.40
1:C:494:GLN:HG3	1:C:497:GLN:NE2	2.36	0.40
1:D:441:MET:HE3	1:D:441:MET:HA	2.02	0.40
1:C:350:ALA:O	1:C:351:ASP:HB3	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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%)	262 (81%)	44 (14%)	18 (6%)	2	6
1	B	318/342 (93%)	281 (88%)	31 (10%)	6 (2%)	10	32
1	C	328/342 (96%)	251 (76%)	61 (19%)	16 (5%)	3	8
1	D	328/342 (96%)	276 (84%)	38 (12%)	14 (4%)	3	10
1	E	328/342 (96%)	291 (89%)	28 (8%)	9 (3%)	6	21
All	All	1626/1710 (95%)	1361 (84%)	202 (12%)	63 (4%)	4	12

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	215	ARG
1	A	252	VAL
1	A	366	ASP
1	A	447	GLU
1	B	235	SER
1	B	386	ASP
1	D	252	VAL
1	D	253	MET
1	D	449	LYS
1	E	215	ARG
1	E	366	ASP
1	A	185	THR
1	A	253	MET
1	A	323	THR
1	A	363	ASP
1	A	365	ILE
1	A	386	ASP
1	A	436	PRO

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Mol	Chain	Res	Type
1	A	448	GLN
1	A	457	ARG
1	A	483	LEU
1	B	185	THR
1	B	188	GLY
1	C	252	VAL
1	C	318	MET
1	C	362	THR
1	C	377	ARG
1	C	419	GLY
1	D	186	THR
1	D	187	SER
1	D	190	GLY
1	E	271	GLY
1	E	498	GLN
1	A	387	SER
1	A	394	GLU
1	B	186	THR
1	C	386	ASP
1	C	389	ASN
1	C	460	SER
1	C	477	ALA
1	D	189	SER
1	D	369	PRO
1	E	483	LEU
1	A	355	ALA
1	B	252	VAL
1	C	367	ILE
1	D	325	GLY
1	D	431	LEU
1	D	455	PRO
1	D	460	SER
1	E	252	VAL
1	C	433	PRO
1	C	473	GLU
1	E	253	MET
1	A	446	CYS
1	C	332	ARG
1	D	447	GLU
1	E	369	PRO
1	C	436	PRO
1	E	433	PRO

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Mol	Chain	Res	Type
1	C	444	VAL
1	D	388	ILE
1	C	188	GLY

### 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%)	264 (94%)	17 (6%)	24	56
1	B	278/294 (95%)	252 (91%)	26 (9%)	11	31
1	C	282/294 (96%)	256 (91%)	26 (9%)	11	32
1	D	282/294 (96%)	255 (90%)	27 (10%)	10	29
1	E	282/294 (96%)	256 (91%)	26 (9%)	11	32
All	All	1405/1470 (96%)	1283 (91%)	122 (9%)	13	35

All (122) 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	267	ASN
1	A	269	ASP
1	A	270	ASN
1	A	307	LEU
1	A	334	LEU
1	A	341	VAL
1	A	346	THR
1	A	364	THR
1	A	382	GLU
1	A	457	ARG
1	A	458	TRP
1	A	472	ARG
1	A	486	LEU

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Mol	Chain	Res	Type
1	A	491	THR
1	B	199	ARG
1	B	204	THR
1	B	209	GLU
1	B	229	VAL
1	B	233	ILE
1	B	238	GLU
1	B	250	GLN
1	B	255	ARG
1	B	269	ASP
1	B	272	THR
1	B	278	LEU
1	B	292	LEU
1	B	294	ARG
1	B	307	LEU
1	B	334	LEU
1	B	341	VAL
1	B	342	LYS
1	B	346	THR
1	B	356	VAL
1	B	382	GLU
1	B	391	LYS
1	B	432	VAL
1	B	464	LEU
1	B	486	LEU
1	B	491	THR
1	B	492	LEU
1	C	177	LEU
1	C	195	LEU
1	C	209	GLU
1	C	215	ARG
1	C	216	PHE
1	C	229	VAL
1	C	240	ARG
1	C	241	SER
1	C	244	ARG
1	C	247	GLU
1	C	255	ARG
1	C	278	LEU
1	C	296	THR
1	C	297	VAL
1	C	326	LYS

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Mol	Chain	Res	Type
1	C	334	LEU
1	C	356	VAL
1	C	364	THR
1	C	379	MET
1	C	382	GLU
1	C	389	ASN
1	C	392	HIS
1	C	414	ARG
1	C	446	CYS
1	C	478	ASN
1	C	483	LEU
1	D	195	LEU
1	D	196	LEU
1	D	204	THR
1	D	209	GLU
1	D	216	PHE
1	D	229	VAL
1	D	231	VAL
1	D	244	ARG
1	D	269	ASP
1	D	272	THR
1	D	278	LEU
1	D	292	LEU
1	D	307	LEU
1	D	321	VAL
1	D	334	LEU
1	D	341	VAL
1	D	342	LYS
1	D	376	LYS
1	D	382	GLU
1	D	389	ASN
1	D	417	ILE
1	D	431	LEU
1	D	432	VAL
1	D	461	CYS
1	D	486	LEU
1	D	491	THR
1	D	492	LEU
1	E	171	ILE
1	E	178	LYS
1	E	204	THR
1	E	209	GLU

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Mol	Chain	Res	Type
1	E	215	ARG
1	E	229	VAL
1	E	238	GLU
1	E	257	GLU
1	E	267	ASN
1	E	278	LEU
1	E	284	GLU
1	E	292	LEU
1	E	307	LEU
1	E	324	GLN
1	E	342	LYS
1	E	356	VAL
1	E	364	THR
1	E	376	LYS
1	E	382	GLU
1	E	389	ASN
1	E	404	MET
1	E	442	ARG
1	E	451	ARG
1	E	456	ASN
1	E	491	THR
1	E	497	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	250	GLN
1	A	267	ASN
1	A	270	ASN
1	A	331	HIS
1	A	448	GLN
1	B	250	GLN
1	B	256	HIS
1	B	258	ASN
1	B	315	HIS
1	B	331	HIS
1	B	389	ASN
1	B	421	HIS
1	B	459	GLN
1	C	208	GLN
1	C	250	GLN
1	C	256	HIS

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Mol	Chain	Res	Type
1	C	258	ASN
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	497	GLN
1	D	250	GLN
1	D	256	HIS
1	D	258	ASN
1	D	293	ASN
1	D	315	HIS
1	D	324	GLN
1	D	331	HIS
1	D	370	ASN
1	D	389	ASN
1	D	392	HIS
1	D	425	GLN
1	D	459	GLN
1	D	497	GLN
1	E	250	GLN
1	E	256	HIS
1	E	258	ASN
1	E	315	HIS
1	E	324	GLN
1	E	331	HIS
1	E	370	ASN
1	E	389	ASN
1	E	448	GLN
1	E	459	GLN
1	E	478	ASN
1	E	497	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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$
2	JZO	A	1	-	25,30,30	1.49	6 (24%)	35,43,43	1.49	7 (20%)
3	PO4	A	21	-	4,4,4	1.09	0	6,6,6	0.27	0
3	PO4	A	22	-	4,4,4	1.14	0	6,6,6	0.27	0
3	PO4	A	9	-	4,4,4	1.16	0	6,6,6	0.27	0
3	PO4	B	11	-	4,4,4	1.13	0	6,6,6	0.27	0
3	PO4	B	12	-	4,4,4	1.19	0	6,6,6	0.27	0
2	JZO	B	2	-	25,30,30	1.47	6 (24%)	35,43,43	1.45	6 (17%)
3	PO4	B	6	-	4,4,4	1.01	0	6,6,6	0.27	0
3	PO4	C	10	-	4,4,4	1.07	0	6,6,6	0.27	0
2	JZO	C	3	-	25,30,30	1.43	5 (20%)	35,43,43	1.53	8 (22%)
3	PO4	D	13	-	4,4,4	1.13	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	15	-	4,4,4	1.27	0	6,6,6	0.27	0
2	JZO	D	4	-	25,30,30	1.54	7 (28%)	35,43,43	1.48	8 (22%)
3	PO4	E	1	-	4,4,4	1.13	0	6,6,6	0.27	0
3	PO4	E	2	-	4,4,4	1.18	0	6,6,6	0.27	0
3	PO4	E	3	-	4,4,4	1.22	0	6,6,6	0.27	0
2	JZO	E	5	-	25,30,30	1.49	5 (20%)	35,43,43	1.55	7 (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
2	JZO	A	1	-	-	0/11/11/11	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PO4	A	21	-	-	0/0/0/0	0/0/0/0
3	PO4	A	22	-	-	0/0/0/0	0/0/0/0
3	PO4	A	9	-	-	0/0/0/0	0/0/0/0
3	PO4	B	11	-	-	0/0/0/0	0/0/0/0
3	PO4	B	12	-	-	0/0/0/0	0/0/0/0
2	JZO	B	2	-	-	0/11/11/11	0/4/4/4
3	PO4	B	6	-	-	0/0/0/0	0/0/0/0
3	PO4	C	10	-	-	0/0/0/0	0/0/0/0
2	JZO	C	3	-	-	0/11/11/11	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	15	-	-	0/0/0/0	0/0/0/0
2	JZO	D	4	-	-	0/11/11/11	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	3	-	-	0/0/0/0	0/0/0/0
2	JZO	E	5	-	-	0/11/11/11	0/4/4/4

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4	JZO	C6-C5	2.01	1.43	1.38
2	B	2	JZO	C19-C18	2.04	1.43	1.39
2	A	1	JZO	C6-C7	2.04	1.43	1.38
2	C	3	JZO	C24-N25	2.05	1.36	1.32
2	C	3	JZO	C19-C18	2.06	1.43	1.39
2	B	2	JZO	C27-C18	2.08	1.43	1.38
2	A	1	JZO	C27-C18	2.09	1.43	1.38
2	E	5	JZO	C19-C18	2.09	1.43	1.39
2	B	2	JZO	C6-C7	2.14	1.43	1.38
2	C	3	JZO	C27-C18	2.14	1.43	1.38
2	A	1	JZO	C7-C8	2.17	1.44	1.39
2	D	4	JZO	C5-C4	2.17	1.43	1.38
2	E	5	JZO	C27-C18	2.19	1.43	1.38
2	A	1	JZO	C5-C4	2.22	1.43	1.38
2	E	5	JZO	C7-C8	2.23	1.44	1.39
2	A	1	JZO	C23-N22	2.23	1.37	1.32
2	D	4	JZO	C6-C7	2.24	1.43	1.38
2	B	2	JZO	C7-C8	2.25	1.44	1.39
2	D	4	JZO	C27-C18	2.27	1.43	1.38
2	D	4	JZO	C7-C8	2.36	1.44	1.39
2	B	2	JZO	C23-N22	2.37	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	JZO	C23-N22	2.38	1.37	1.32
2	D	4	JZO	C23-N22	2.47	1.37	1.32
2	E	5	JZO	C23-N22	2.71	1.38	1.32
2	C	3	JZO	C20-C19	2.94	1.42	1.36
2	B	2	JZO	C20-C19	2.96	1.42	1.36
2	E	5	JZO	C20-C19	2.99	1.42	1.36
2	A	1	JZO	C20-C19	3.09	1.43	1.36
2	D	4	JZO	C20-C19	3.32	1.43	1.36

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	5	JZO	C15-N14-C16	-3.76	124.52	129.59
2	C	3	JZO	C15-N14-C16	-3.67	124.65	129.59
2	A	1	JZO	C15-N14-C16	-3.51	124.86	129.59
2	B	2	JZO	C15-N14-C16	-3.46	124.94	129.59
2	D	4	JZO	C15-N14-C16	-2.93	125.65	129.59
2	E	5	JZO	C26-C21-N22	-2.91	118.33	121.02
2	A	1	JZO	C26-C21-N22	-2.81	118.42	121.02
2	C	3	JZO	C26-C21-N22	-2.75	118.48	121.02
2	D	4	JZO	C26-C21-N22	-2.72	118.50	121.02
2	B	2	JZO	C26-C21-N22	-2.70	118.52	121.02
2	D	4	JZO	C24-C23-N22	-2.17	118.56	122.84
2	E	5	JZO	C24-C23-N22	-2.09	118.72	122.84
2	C	3	JZO	C24-C23-N22	-2.08	118.73	122.84
2	C	3	JZO	C21-C26-N25	-2.02	119.16	121.02
2	D	4	JZO	C21-C26-N25	-2.01	119.16	121.02
2	A	1	JZO	C24-C23-N22	-2.01	118.88	122.84
2	B	2	JZO	C15-N14-N12	2.00	125.44	121.95
2	A	1	JZO	C15-N14-N12	2.02	125.48	121.95
2	D	4	JZO	C8-C10-C11	2.04	130.92	126.88
2	C	3	JZO	C15-N14-N12	2.20	125.79	121.95
2	E	5	JZO	C15-N14-N12	2.24	125.85	121.95
2	B	2	JZO	C27-C26-N25	2.45	120.65	117.95
2	A	1	JZO	C27-C26-N25	2.48	120.69	117.95
2	E	5	JZO	C27-C26-N25	2.61	120.83	117.95
2	D	4	JZO	C27-C26-N25	2.68	120.91	117.95
2	C	3	JZO	C24-N25-C26	2.68	121.41	116.87
2	C	3	JZO	C27-C26-N25	2.70	120.93	117.95
2	A	1	JZO	C24-N25-C26	2.81	121.64	116.87
2	B	2	JZO	C24-N25-C26	2.86	121.72	116.87
2	D	4	JZO	C24-N25-C26	2.94	121.85	116.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	JZO	C23-N22-C21	3.01	121.98	116.87
2	E	5	JZO	C24-N25-C26	3.07	122.07	116.87
2	A	1	JZO	C23-N22-C21	3.19	122.27	116.87
2	E	5	JZO	C23-N22-C21	3.19	122.28	116.87
2	D	4	JZO	C23-N22-C21	3.25	122.38	116.87
2	C	3	JZO	C23-N22-C21	3.32	122.50	116.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	JZO	1	0
3	B	11	PO4	2	0
3	B	12	PO4	1	0
3	B	6	PO4	1	0
3	C	10	PO4	1	0
2	C	3	JZO	3	0
3	D	14	PO4	1	0
3	D	15	PO4	2	0
2	D	4	JZO	3	0
3	E	2	PO4	2	0
3	E	3	PO4	3	0
2	E	5	JZO	1	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%)	0.48	29 (8%) 12 6	23, 67, 105, 113	0
1	B	324/342 (94%)	-0.04	6 (1%) 70 59	17, 38, 68, 98	0
1	C	330/342 (96%)	0.64	40 (12%) 6 3	21, 71, 100, 110	0
1	D	330/342 (96%)	0.09	15 (4%) 37 26	20, 43, 82, 93	0
1	E	330/342 (96%)	0.01	13 (3%) 43 31	18, 37, 76, 93	0
All	All	1642/1710 (96%)	0.24	103 (6%) 23 14	17, 47, 96, 113	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	324	GLN	6.0
1	C	252	VAL	5.9
1	C	497	GLN	5.4
1	D	323	THR	5.4
1	E	370	ASN	4.9
1	B	191	SER	4.8
1	A	323	THR	4.7
1	C	322	GLY	4.7
1	B	252	VAL	4.7
1	D	190	GLY	4.6
1	C	369	PRO	4.6
1	A	325	GLY	4.5
1	C	323	THR	4.5
1	E	323	THR	4.4
1	E	325	GLY	4.4
1	A	416	SER	4.3
1	C	187	SER	4.3
1	D	325	GLY	4.1
1	D	189	SER	4.0
1	C	462	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	190	GLY	4.0
1	A	253	MET	3.9
1	A	322	GLY	3.9
1	C	496	SER	3.9
1	C	455	PRO	3.8
1	A	432	VAL	3.8
1	E	188	GLY	3.7
1	C	443	LYS	3.6
1	A	417	ILE	3.6
1	D	419	GLY	3.6
1	A	189	SER	3.5
1	E	189	SER	3.5
1	D	322	GLY	3.5
1	A	446	CYS	3.4
1	A	191	SER	3.4
1	B	188	GLY	3.3
1	E	324	GLN	3.3
1	C	291	TYR	3.3
1	D	370	ASN	3.3
1	C	321	VAL	3.3
1	A	431	LEU	3.2
1	C	325	GLY	3.1
1	C	416	SER	3.1
1	A	499	GLU	3.1
1	D	324	GLN	3.1
1	C	361	ALA	3.0
1	C	253	MET	3.0
1	A	321	VAL	3.0
1	A	443	LYS	3.0
1	C	370	ASN	2.9
1	E	187	SER	2.8
1	E	253	MET	2.8
1	C	411	ILE	2.8
1	C	417	ILE	2.8
1	D	188	GLY	2.8
1	C	324	GLN	2.8
1	C	360	SER	2.7
1	D	191	SER	2.7
1	E	321	VAL	2.7
1	C	434	SER	2.7
1	A	457	ARG	2.7
1	C	465	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	428	TYR	2.7
1	E	322	GLY	2.6
1	A	458	TRP	2.6
1	A	433	PRO	2.6
1	C	460	SER	2.6
1	A	216	PHE	2.6
1	C	320	ILE	2.5
1	C	424	TYR	2.5
1	A	295	TYR	2.4
1	C	318	MET	2.4
1	C	188	GLY	2.4
1	C	421	HIS	2.4
1	C	392	HIS	2.4
1	C	420	ILE	2.4
1	D	252	VAL	2.4
1	E	252	VAL	2.4
1	C	498	GLN	2.4
1	C	300	GLU	2.4
1	E	216	PHE	2.2
1	A	447	GLU	2.2
1	C	299	VAL	2.2
1	E	190	GLY	2.2
1	C	433	PRO	2.2
1	C	458	TRP	2.2
1	C	295	TYR	2.2
1	C	494	GLN	2.2
1	C	463	ALA	2.2
1	B	253	MET	2.1
1	D	216	PHE	2.1
1	A	448	GLN	2.1
1	A	292	LEU	2.1
1	A	294	ARG	2.1
1	D	418	GLY	2.1
1	A	320	ILE	2.1
1	B	391	LYS	2.1
1	C	470	ILE	2.1
1	D	462	GLU	2.1
1	D	439	GLU	2.0
1	A	442	ARG	2.0
1	A	418	GLY	2.0
1	B	325	GLY	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	15	5/5	0.94	0.34	4.43	2,7,8,8	5
3	PO4	D	14	5/5	0.95	0.32	4.23	21,21,21,22	5
3	PO4	E	2	5/5	0.98	0.23	2.58	7,8,10,11	5
3	PO4	B	12	5/5	0.98	0.20	1.76	15,16,16,18	5
3	PO4	E	3	5/5	0.98	0.25	1.58	1,1,2,3	5
2	JZO	E	5	27/27	0.97	0.19	0.90	25,28,32,32	0
2	JZO	A	1	27/27	0.98	0.21	0.84	26,30,34,39	0
2	JZO	D	4	27/27	0.97	0.20	0.81	25,28,35,39	0
3	PO4	B	11	5/5	0.97	0.24	0.76	1,2,6,6	5
2	JZO	C	3	27/27	0.96	0.21	0.64	41,47,49,50	0
2	JZO	B	2	27/27	0.98	0.17	-0.04	17,22,26,30	0
3	PO4	A	22	5/5	0.93	0.23	-0.25	19,20,22,23	5
3	PO4	A	21	5/5	0.94	0.22	-0.41	35,36,36,37	5
3	PO4	D	13	5/5	0.97	0.14	-0.75	54,54,55,56	0
3	PO4	B	6	5/5	0.95	0.15	-1.03	37,37,38,40	0
3	PO4	E	1	5/5	0.97	0.15	-1.03	44,44,46,46	0
3	PO4	A	9	5/5	0.94	0.16	-1.05	69,70,70,71	0
3	PO4	C	10	5/5	0.89	0.18	-1.50	61,61,63,63	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.