



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:00 PM GMT

PDB ID : 3SCK  
Title : Crystal structure of spike protein receptor-binding domain from a predicted SARS coronavirus civet strain complexed with human-civet chimeric receptor ACE2  
Authors : Wu, K.; Peng, G.; Wilken, M.; Geraghty, R.; Li, F.  
Deposited on : 2011-06-07  
Resolution : 3.00 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

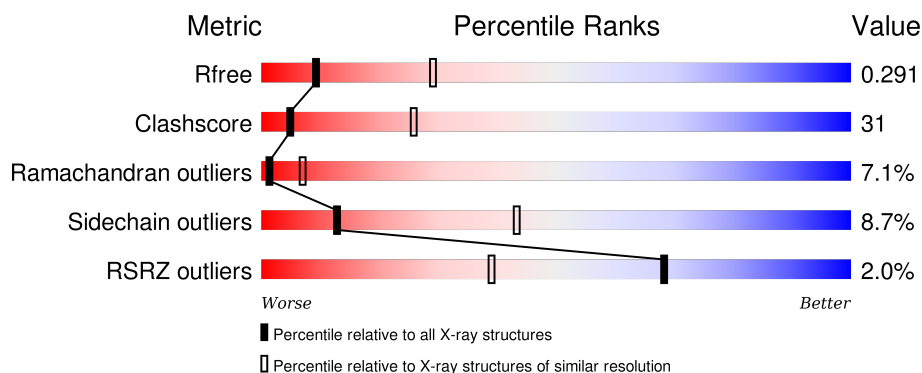
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	603	
1	B	603	
2	E	185	
2	F	185	

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
4	CL	A	902	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12518 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 Angiotensin-converting enzyme 2 chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	597	Total	C	N	O	S	0	0	0
			4863	3109	803	923	28			
1	B	597	Total	C	N	O	S	0	0	0
			4863	3109	803	923	28			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	616	HIS	-	EXPRESSION TAG	UNP Q9BYF1
A	617	HIS	-	EXPRESSION TAG	UNP Q9BYF1
A	618	HIS	-	EXPRESSION TAG	UNP Q9BYF1
A	619	HIS	-	EXPRESSION TAG	UNP Q9BYF1
A	620	HIS	-	EXPRESSION TAG	UNP Q9BYF1
A	621	HIS	-	EXPRESSION TAG	UNP Q9BYF1
B	616	HIS	-	EXPRESSION TAG	UNP Q9BYF1
B	617	HIS	-	EXPRESSION TAG	UNP Q9BYF1
B	618	HIS	-	EXPRESSION TAG	UNP Q9BYF1
B	619	HIS	-	EXPRESSION TAG	UNP Q9BYF1
B	620	HIS	-	EXPRESSION TAG	UNP Q9BYF1
B	621	HIS	-	EXPRESSION TAG	UNP Q9BYF1

- Molecule 2 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	173	Total	C	N	O	S	0	0	0
			1394	905	229	254	6			
2	F	173	Total	C	N	O	S	0	0	0
			1394	905	229	254	6			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	472	PRO	LEU	SEE REMARK 999	UNP P59594
E	479	ARG	ASN	CONFLICT	UNP P59594
E	480	GLY	ASP	SEE REMARK 999	UNP P59594
E	503	HIS	-	EXPRESSION TAG	UNP P59594
E	504	HIS	-	EXPRESSION TAG	UNP P59594
E	505	HIS	-	EXPRESSION TAG	UNP P59594
E	506	HIS	-	EXPRESSION TAG	UNP P59594
E	507	HIS	-	EXPRESSION TAG	UNP P59594
E	508	HIS	-	EXPRESSION TAG	UNP P59594
F	472	PRO	LEU	SEE REMARK 999	UNP P59594
F	479	ARG	ASN	CONFLICT	UNP P59594
F	480	GLY	ASP	SEE REMARK 999	UNP P59594
F	503	HIS	-	EXPRESSION TAG	UNP P59594
F	504	HIS	-	EXPRESSION TAG	UNP P59594
F	505	HIS	-	EXPRESSION TAG	UNP P59594
F	506	HIS	-	EXPRESSION TAG	UNP P59594
F	507	HIS	-	EXPRESSION TAG	UNP P59594
F	508	HIS	-	EXPRESSION TAG	UNP P59594

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Zn 1 1	0	0
3	A	1	Total Zn 1 1	0	0

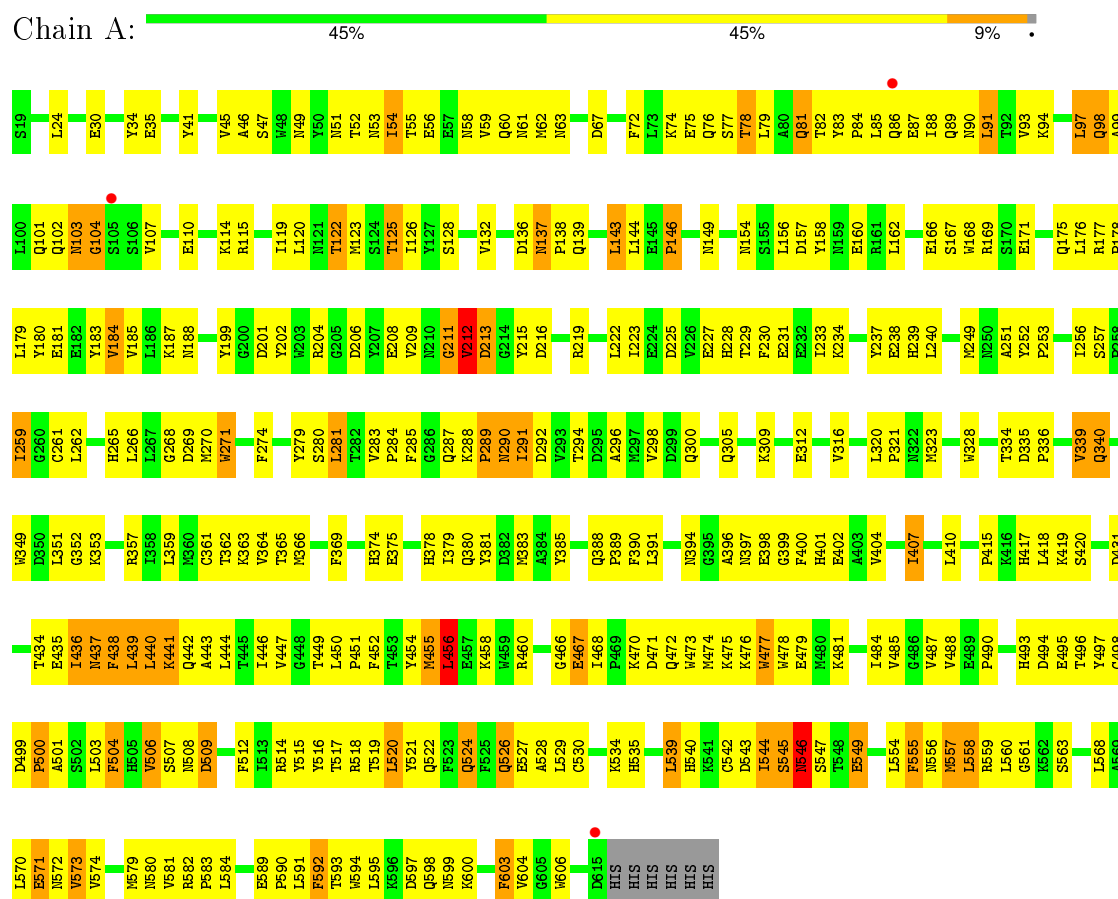
- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0
4	A	1	Total Cl 1 1	0	0

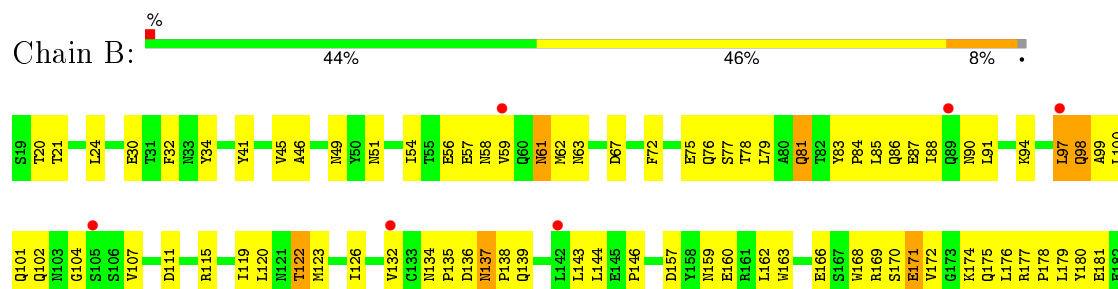
### 3 Residue-property plots

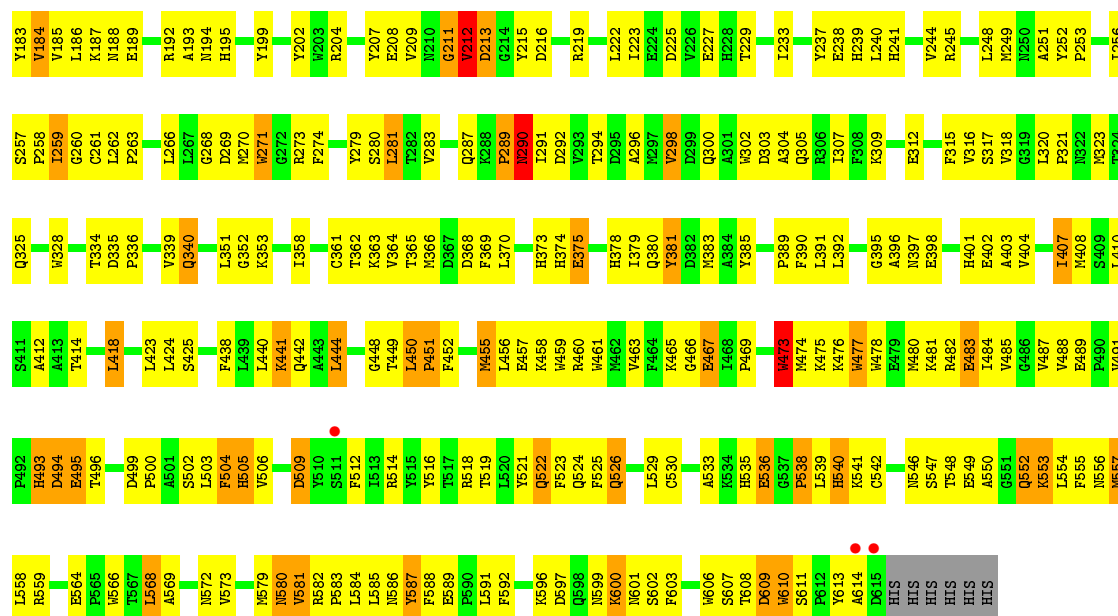
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ( $\text{RSRZ} > 2$ ). 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: Angiotensin-converting enzyme 2 chimera

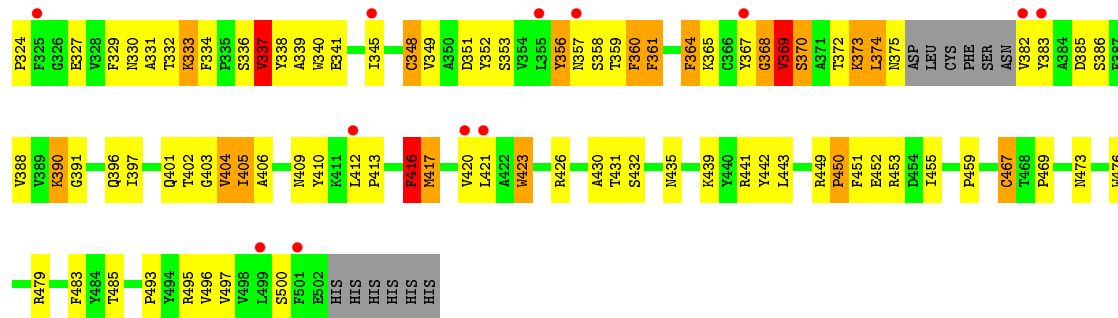


- Molecule 1: Angiotensin-converting enzyme 2 chimera

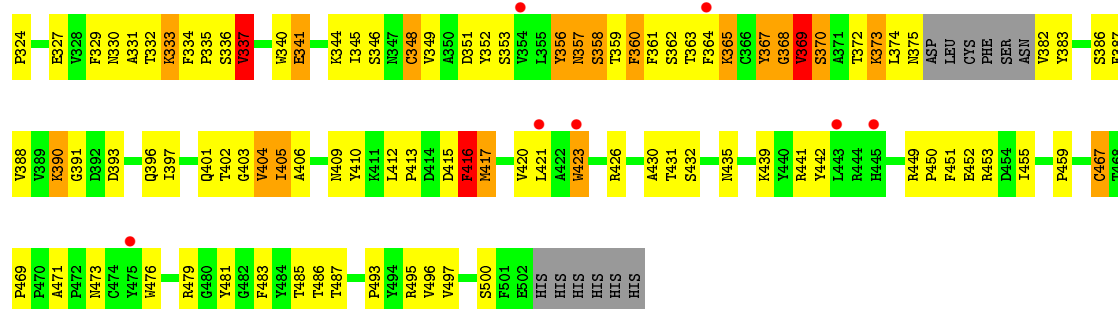
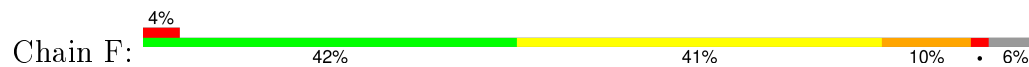




### • Molecule 2: Spike glycoprotein



### • Molecule 2: Spike glycoprotein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.22Å 119.28Å 113.24Å 90.00° 92.19° 90.00°	Depositor
Resolution (Å)	47.27 – 3.00 47.27 – 2.99	Depositor EDS
% Data completeness (in resolution range)	78.7 (47.27-3.00) 76.8 (47.27-2.99)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.16 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.239 , 0.285 0.245 , 0.291	Depositor DCC
$R_{free}$ test set	2141 reflections (6.70%)	DCC
Wilson B-factor (Å <sup>2</sup> )	84.7	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 48.3	EDS
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 42932 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12518	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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: ZN, CL

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	0.57	0/4999	0.67	2/6796 (0.0%)
1	B	0.55	0/4999	0.64	0/6796
2	E	0.60	0/1440	0.65	0/1961
2	F	0.57	0/1440	0.62	0/1961
All	All	0.56	0/12878	0.65	2/17514 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	290	ASN	N-CA-C	5.38	125.52	111.00
1	A	291	ILE	N-CA-C	-5.22	96.91	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	4863	0	4636	297	0
1	B	4863	0	4636	319	0
2	E	1394	0	1327	73	0
2	F	1394	0	1327	85	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	12518	0	11926	765	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 (765) 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)
2:E:324:PRO:HG3	2:E:348:CYS:SG	1.87	1.12
1:A:456:LEU:HD22	1:A:477:TRP:HH2	1.16	1.03
2:F:324:PRO:HG3	2:F:348:CYS:SG	2.01	1.00
1:B:582:ARG:HB3	1:B:583:PRO:HD3	1.46	0.97
1:A:410:LEU:HD23	1:A:526:GLN:HG3	1.46	0.97
1:B:209:VAL:HB	1:B:216:ASP:HA	1.52	0.92
1:B:179:LEU:H	1:B:179:LEU:HD12	1.34	0.92
1:B:143:LEU:HD13	1:B:144:LEU:H	1.35	0.91
1:B:533:ALA:HB2	1:B:550:ALA:HB2	1.53	0.90
1:A:143:LEU:HD13	1:A:144:LEU:H	1.35	0.90
1:B:177:ARG:HH12	1:B:495:GLU:HG3	1.39	0.88
1:B:289:PRO:O	1:B:290:ASN:O	1.92	0.86
1:B:483:GLU:HB3	1:B:608:THR:HG22	1.58	0.86
1:B:485:VAL:HG12	1:B:487:VAL:HG23	1.58	0.86
1:A:179:LEU:H	1:A:179:LEU:HD12	1.40	0.85
2:E:409:ASN:HD21	2:E:441:ARG:H	1.24	0.85
1:A:456:LEU:HD22	1:A:477:TRP:CH2	2.08	0.85
1:A:132:VAL:HG12	1:A:171:GLU:HG3	1.58	0.85
1:B:99:ALA:O	1:B:102:GLN:HG3	1.76	0.84
2:F:327:GLU:O	2:F:331:ALA:HB2	1.80	0.82
1:A:97:LEU:O	1:A:101:GLN:HG2	1.80	0.81
2:F:388:VAL:HG22	2:F:495:ARG:HG2	1.60	0.81
2:F:426:ARG:O	2:F:430:ALA:HB3	1.82	0.80
1:A:543:ASP:OD1	1:A:545:SER:HB2	1.81	0.80
1:B:143:LEU:HD13	1:B:144:LEU:N	1.98	0.79
1:B:478:TRP:O	1:B:482:ARG:HB2	1.82	0.79
1:B:397:ASN:HD22	1:B:566:TRP:HB2	1.46	0.77
1:A:501:ALA:O	1:A:507:SER:HB3	1.84	0.77
1:A:520:LEU:HD22	1:A:520:LEU:H	1.50	0.77
1:B:296:ALA:O	1:B:300:GLN:HG3	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:GLN:HE21	1:B:81:GLN:HA	1.51	0.76
1:A:309:LYS:HD2	1:A:328:TRP:CH2	2.19	0.76
1:B:549:GLU:CD	1:B:549:GLU:H	1.89	0.76
1:B:397:ASN:HD22	1:B:566:TRP:CB	1.99	0.75
1:A:557:MET:O	1:A:557:MET:HE2	1.87	0.74
2:E:336:SER:OG	2:E:439:LYS:N	2.21	0.74
1:A:274:PHE:CD2	1:A:449:THR:HB	2.23	0.74
1:A:252:TYR:CE2	1:A:266:LEU:HD22	2.22	0.74
1:A:441:LYS:HG3	1:A:441:LYS:O	1.86	0.74
1:A:603:PHE:HD2	1:A:604:VAL:N	1.85	0.74
1:A:85:LEU:HD12	1:A:85:LEU:H	1.53	0.73
1:B:325:GLN:HE22	2:F:426:ARG:NH2	1.87	0.73
2:E:388:VAL:HG22	2:E:495:ARG:HG2	1.71	0.73
1:A:400:PHE:HD2	1:A:557:MET:HE1	1.51	0.73
1:A:72:PHE:O	1:A:76:GLN:HG2	1.89	0.73
2:F:353:SER:HA	2:F:356:TYR:HB2	1.71	0.72
1:A:143:LEU:HD13	1:A:144:LEU:N	2.04	0.72
1:B:229:THR:HG23	1:B:516:TYR:OH	1.88	0.72
1:B:225:ASP:O	1:B:229:THR:HG22	1.90	0.72
2:F:336:SER:OG	2:F:439:LYS:N	2.22	0.72
1:B:438:PHE:O	1:B:442:GLN:HG2	1.90	0.72
1:B:459:TRP:O	1:B:463:VAL:HG23	1.89	0.72
2:F:452:GLU:HG2	2:F:453:ARG:H	1.55	0.71
2:E:426:ARG:O	2:E:430:ALA:HB3	1.89	0.71
2:E:390:LYS:HG2	2:E:391:GLY:N	2.05	0.71
1:B:30:GLU:O	1:B:34:TYR:HD1	1.73	0.71
1:B:136:ASP:O	1:B:137:ASN:HB2	1.90	0.71
1:B:177:ARG:NH1	1:B:495:GLU:HG3	2.05	0.71
2:E:390:LYS:HG2	2:E:391:GLY:H	1.54	0.71
1:A:524:GLN:HE22	1:A:579:MET:HA	1.55	0.71
2:E:324:PRO:CG	2:E:348:CYS:SG	2.76	0.70
2:F:388:VAL:CG2	2:F:495:ARG:HG2	2.22	0.70
1:B:483:GLU:OE2	1:B:484:ILE:HG13	1.91	0.70
1:B:294:THR:HG23	1:B:365:THR:HA	1.72	0.70
1:A:478:TRP:HA	1:A:481:LYS:HB2	1.73	0.69
1:B:24:LEU:HD22	2:F:473:ASN:HD22	1.58	0.69
1:A:528:ALA:HB2	1:A:574:VAL:HA	1.75	0.69
1:A:225:ASP:O	1:A:229:THR:HG22	1.92	0.69
1:A:471:ASP:HA	1:A:495:GLU:HG3	1.74	0.69
1:A:573:VAL:HG23	1:A:574:VAL:H	1.58	0.69
1:B:581:VAL:O	1:B:585:LEU:HD23	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:PHE:O	1:B:76:GLN:HG2	1.93	0.68
1:B:474:MET:C	1:B:476:LYS:H	1.96	0.68
1:A:294:THR:HG23	1:A:365:THR:HA	1.74	0.68
1:B:378:HIS:CE1	1:B:402:GLU:OE1	2.47	0.68
1:A:543:ASP:O	1:A:545:SER:N	2.27	0.68
1:A:519:THR:O	1:A:522:GLN:HG2	1.94	0.68
1:B:252:TYR:CE2	1:B:266:LEU:HD22	2.29	0.67
1:A:549:GLU:H	1:A:549:GLU:CD	1.97	0.67
1:B:463:VAL:HG13	1:B:473:TRP:HE1	1.59	0.67
1:A:81:GLN:HE21	1:A:81:GLN:HA	1.59	0.67
1:B:227:GLU:OE2	1:B:458:LYS:HE2	1.94	0.67
1:B:166:GLU:OE2	1:B:493:HIS:HE1	1.78	0.66
1:B:483:GLU:HB3	1:B:608:THR:CG2	2.25	0.66
1:A:400:PHE:CD2	1:A:557:MET:HE1	2.30	0.66
1:B:455:MET:SD	1:B:481:LYS:HG2	2.36	0.66
1:A:539:LEU:HD12	1:A:539:LEU:O	1.96	0.66
1:A:597:ASP:O	1:A:600:LYS:HG2	1.96	0.66
2:F:406:ALA:HA	2:F:410:TYR:O	1.97	0.65
1:B:223:ILE:O	1:B:227:GLU:HG3	1.96	0.65
1:B:294:THR:O	1:B:298:VAL:HG23	1.95	0.65
1:B:180:TYR:O	1:B:184:VAL:HG23	1.96	0.65
2:E:420:VAL:C	2:E:421:LEU:HD12	2.17	0.65
2:F:334:PHE:CE2	2:F:386:SER:HB2	2.31	0.65
1:B:175:GLN:O	1:B:178:PRO:HD2	1.97	0.65
1:A:474:MET:CE	1:A:499:ASP:H	2.10	0.64
1:B:211:GLY:O	1:B:212:VAL:HG13	1.96	0.64
1:A:296:ALA:O	1:A:300:GLN:HG3	1.96	0.64
1:A:557:MET:SD	1:A:558:LEU:HD12	2.38	0.64
1:A:102:GLN:C	1:A:104:GLY:H	2.00	0.64
1:B:378:HIS:NE2	1:B:402:GLU:OE1	2.30	0.64
1:B:21:THR:HG21	1:B:87:GLU:OE1	1.98	0.64
1:A:274:PHE:HD2	1:A:449:THR:HB	1.63	0.64
1:A:320:LEU:HB3	1:A:321:PRO:HD2	1.77	0.64
1:A:516:TYR:CE2	1:A:520:LEU:HD21	2.33	0.64
1:B:582:ARG:HB3	1:B:583:PRO:CD	2.26	0.63
2:F:324:PRO:CG	2:F:348:CYS:SG	2.84	0.63
1:A:233:ILE:HG12	1:A:581:VAL:HG21	1.80	0.63
1:A:30:GLU:O	1:A:34:TYR:HD1	1.82	0.63
1:A:493:HIS:HD2	1:A:499:ASP:OD1	1.80	0.63
1:B:581:VAL:HG22	1:B:585:LEU:CD2	2.28	0.63
1:B:177:ARG:O	1:B:181:GLU:HG3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:VAL:HA	1:B:547:SER:O	1.99	0.62
1:A:339:VAL:O	1:A:340:GLN:HB2	1.99	0.62
1:B:107:VAL:HG21	1:B:193:ALA:HB1	1.81	0.62
1:A:132:VAL:HG12	1:A:171:GLU:CG	2.29	0.62
2:F:351:ASP:O	2:F:352:TYR:HB2	1.98	0.62
1:B:261:CYS:HB2	1:B:488:VAL:HG13	1.81	0.62
1:B:259:ILE:O	1:B:259:ILE:HG13	2.00	0.62
2:E:396:GLN:OE1	2:E:405:ILE:HB	1.99	0.62
1:A:204:ARG:HD2	1:A:219:ARG:O	1.98	0.62
1:B:457:GLU:HG2	1:B:512:PHE:HB3	1.82	0.62
2:E:329:PHE:C	2:E:331:ALA:H	2.02	0.62
1:A:446:ILE:H	1:A:446:ILE:HD12	1.65	0.62
1:A:474:MET:HE2	1:A:499:ASP:H	1.65	0.62
1:B:609:ASP:OD2	1:B:609:ASP:N	2.32	0.62
1:B:541:LYS:HE2	1:B:541:LYS:HA	1.82	0.62
1:A:434:THR:O	1:A:437:ASN:HB2	1.99	0.62
1:A:136:ASP:O	1:A:137:ASN:HB2	2.00	0.62
1:B:440:LEU:HD13	1:B:444:LEU:HD22	1.82	0.61
2:F:390:LYS:HG2	2:F:391:GLY:H	1.65	0.61
1:B:233:ILE:HD13	1:B:450:LEU:HD23	1.80	0.61
1:A:388:GLN:OE1	1:A:563:SER:HB2	2.01	0.61
1:A:526:GLN:O	1:A:530:CYS:SG	2.58	0.61
1:A:294:THR:O	1:A:298:VAL:HG23	2.00	0.61
1:B:204:ARG:HD2	1:B:219:ARG:O	2.01	0.61
2:F:417:MET:HA	2:F:417:MET:HE2	1.83	0.61
1:B:477:TRP:CZ3	1:B:500:PRO:HB3	2.35	0.61
2:F:409:ASN:HD21	2:F:441:ARG:H	1.47	0.61
1:B:85:LEU:H	1:B:85:LEU:HD12	1.65	0.61
1:A:439:LEU:HD12	1:A:591:LEU:HB2	1.83	0.60
2:F:390:LYS:HG2	2:F:391:GLY:N	2.16	0.60
1:A:443:ALA:HA	1:A:447:VAL:HG23	1.82	0.60
1:A:454:TYR:OH	1:A:458:LYS:HE3	2.01	0.60
2:E:333:LYS:O	2:E:333:LYS:HD2	2.00	0.60
1:A:98:GLN:O	1:A:101:GLN:HB2	2.01	0.60
1:A:579:MET:HG3	1:A:579:MET:O	2.01	0.60
1:B:63:ASN:O	1:B:67:ASP:N	2.26	0.60
1:A:493:HIS:CD2	1:A:499:ASP:OD1	2.54	0.60
1:B:24:LEU:HD22	2:F:473:ASN:ND2	2.15	0.60
1:A:157:ASP:HB3	1:A:160:GLU:HB3	1.84	0.60
1:B:325:GLN:HE22	2:F:426:ARG:HH22	1.48	0.60
1:B:238:GLU:O	1:B:241:HIS:HB3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:VAL:HB	1:A:216:ASP:HA	1.83	0.59
1:A:503:LEU:O	1:A:506:VAL:HG23	2.02	0.59
1:B:489:GLU:HG2	1:B:613:TYR:HE2	1.67	0.59
2:F:361:PHE:CE1	2:F:421:LEU:HD23	2.38	0.59
1:B:179:LEU:CD1	1:B:179:LEU:H	2.12	0.59
1:A:378:HIS:CE1	1:A:402:GLU:OE1	2.55	0.59
1:A:233:ILE:CG1	1:A:581:VAL:HG21	2.32	0.59
1:A:261:CYS:HB2	1:A:488:VAL:HG13	1.84	0.59
1:B:339:VAL:O	1:B:340:GLN:HB2	2.00	0.59
2:F:373:LYS:HZ2	2:F:375:ASN:HB2	1.67	0.59
1:B:524:GLN:HE22	1:B:579:MET:HA	1.67	0.59
1:B:270:MET:HB3	1:B:271:TRP:CZ3	2.38	0.59
1:B:499:ASP:O	1:B:502:SER:HB3	2.02	0.58
1:A:177:ARG:NH1	1:A:470:LYS:O	2.36	0.58
2:E:329:PHE:O	2:E:331:ALA:N	2.35	0.58
1:B:381:TYR:HE2	1:B:558:LEU:O	1.86	0.58
1:B:132:VAL:HG12	1:B:171:GLU:HG3	1.85	0.58
1:A:176:LEU:HA	1:A:179:LEU:HD13	1.86	0.58
2:F:420:VAL:C	2:F:421:LEU:HD12	2.23	0.58
1:B:457:GLU:CG	1:B:512:PHE:HB3	2.33	0.58
1:A:123:MET:HE3	1:A:183:TYR:CD2	2.39	0.58
1:A:115:ARG:O	1:A:119:ILE:HG12	2.03	0.58
1:B:77:SER:C	1:B:79:LEU:H	2.07	0.58
1:B:81:GLN:CA	1:B:81:GLN:HE21	2.17	0.58
1:B:137:ASN:H	1:B:138:PRO:HD3	1.69	0.58
2:E:373:LYS:HZ2	2:E:375:ASN:HB2	1.69	0.58
1:B:504:PHE:HD2	1:B:505:HIS:N	2.02	0.58
1:B:320:LEU:HB3	1:B:321:PRO:HD2	1.85	0.58
2:E:368:GLY:O	2:E:369:VAL:HG13	2.03	0.58
1:B:493:HIS:HD2	1:B:499:ASP:OD1	1.87	0.57
1:A:312:GLU:O	1:A:316:VAL:HG23	2.03	0.57
2:E:409:ASN:ND2	2:E:441:ARG:H	2.00	0.57
2:E:327:GLU:O	2:E:331:ALA:HB2	2.04	0.57
2:F:397:ILE:O	2:F:420:VAL:HG21	2.03	0.57
2:E:348:CYS:SG	2:E:349:VAL:N	2.77	0.57
2:F:329:PHE:C	2:F:331:ALA:H	2.07	0.57
1:A:259:ILE:O	1:A:606:TRP:HA	2.03	0.57
1:A:455:MET:SD	1:A:481:LYS:HG2	2.45	0.57
1:A:256:ILE:HG22	1:A:257:SER:N	2.18	0.57
1:B:249:MET:HG2	1:B:256:ILE:HB	1.87	0.57
1:A:402:GLU:HB3	1:A:518:ARG:CD	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:580:ASN:C	1:B:582:ARG:H	2.08	0.56
2:E:345:ILE:O	2:E:382:VAL:HG12	2.04	0.56
2:F:413:PRO:HB2	2:F:416:PHE:HD1	1.70	0.56
1:A:374:HIS:C	1:A:374:HIS:CD2	2.77	0.56
2:E:459:PRO:HB3	2:E:467:CYS:HB3	1.87	0.56
1:A:251:ALA:O	1:A:253:PRO:HD3	2.05	0.56
1:B:123:MET:HE3	1:B:183:TYR:CD2	2.41	0.56
1:A:290:ASN:C	1:A:292:ASP:H	2.07	0.56
1:B:582:ARG:HE	1:B:582:ARG:HA	1.70	0.56
1:A:184:VAL:HG12	1:A:188:ASN:HD22	1.70	0.56
2:F:329:PHE:O	2:F:331:ALA:N	2.38	0.56
1:A:591:LEU:O	1:A:593:THR:N	2.38	0.56
2:E:353:SER:HA	2:E:356:TYR:HB2	1.86	0.56
1:B:440:LEU:HD13	1:B:440:LEU:C	2.26	0.56
2:E:383:TYR:HB2	2:E:500:SER:HB2	1.87	0.56
1:A:199:TYR:O	1:A:202:TYR:HB3	2.06	0.56
1:A:77:SER:C	1:A:79:LEU:H	2.08	0.56
1:A:447:VAL:HA	1:A:450:LEU:HD12	1.88	0.55
2:F:368:GLY:O	2:F:369:VAL:HG13	2.06	0.55
1:B:474:MET:C	1:B:476:LYS:N	2.59	0.55
1:A:177:ARG:HD3	1:A:498:CYS:HB2	1.87	0.55
1:A:450:LEU:HB2	1:A:451:PRO:HD3	1.88	0.55
1:A:184:VAL:HG12	1:A:188:ASN:ND2	2.21	0.55
1:A:466:GLY:O	1:A:468:ILE:N	2.39	0.55
1:A:169:ARG:O	1:A:497:TYR:HD1	1.89	0.55
1:B:261:CYS:HB2	1:B:488:VAL:CG1	2.36	0.55
1:B:87:GLU:C	1:B:88:ILE:HD12	2.27	0.55
1:A:400:PHE:HE2	1:A:557:MET:HE3	1.71	0.55
2:F:452:GLU:HG2	2:F:453:ARG:N	2.20	0.55
1:B:363:LYS:O	1:B:365:THR:N	2.40	0.55
1:A:309:LYS:HD2	1:A:328:TRP:CZ2	2.41	0.55
1:B:245:ARG:NH1	1:B:603:PHE:O	2.39	0.55
1:A:589:GLU:H	1:A:590:PRO:CD	2.20	0.55
1:B:251:ALA:O	1:B:253:PRO:HD3	2.07	0.55
1:A:204:ARG:HG2	1:A:222:LEU:HD23	1.87	0.55
2:F:348:CYS:SG	2:F:349:VAL:N	2.80	0.55
1:A:472:GLN:O	1:A:476:LYS:HB2	2.06	0.55
1:A:389:PRO:O	1:A:391:LEU:N	2.39	0.55
1:A:529:LEU:HD23	1:A:544:ILE:HG21	1.88	0.54
1:B:504:PHE:CD2	1:B:505:HIS:N	2.75	0.54
1:A:175:GLN:O	1:A:178:PRO:HD2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:VAL:HG12	1:A:487:VAL:HG23	1.89	0.54
2:F:386:SER:HA	2:F:496:VAL:O	2.07	0.54
1:A:101:GLN:HE21	1:A:101:GLN:HA	1.72	0.54
1:B:487:VAL:HG12	1:B:488:VAL:N	2.22	0.54
2:F:357:ASN:O	2:F:358:SER:HB3	2.07	0.54
1:A:252:TYR:CD2	1:A:266:LEU:HD13	2.43	0.54
1:B:271:TRP:CE2	1:B:503:LEU:HD23	2.42	0.54
1:A:180:TYR:O	1:A:184:VAL:HG23	2.06	0.54
1:B:251:ALA:CB	1:B:281:LEU:HD22	2.38	0.54
2:E:345:ILE:HB	2:E:382:VAL:CG1	2.38	0.54
2:E:403:GLY:O	2:E:404:VAL:HB	2.07	0.54
2:F:335:PRO:HG3	2:F:341:GLU:HB2	1.89	0.54
1:B:474:MET:O	1:B:476:LYS:N	2.41	0.54
1:A:527:GLU:O	1:A:528:ALA:C	2.47	0.54
1:A:435:GLU:O	1:A:439:LEU:HB2	2.08	0.53
2:E:459:PRO:CB	2:E:467:CYS:HB3	2.39	0.53
1:B:374:HIS:CD2	1:B:374:HIS:C	2.81	0.53
2:E:452:GLU:HG2	2:E:453:ARG:H	1.73	0.53
1:A:589:GLU:N	1:A:590:PRO:CD	2.71	0.53
1:B:519:THR:O	1:B:522:GLN:HB3	2.09	0.53
1:A:499:ASP:C	1:A:501:ALA:H	2.12	0.53
1:B:32:PHE:CE2	1:B:100:LEU:HD21	2.43	0.53
1:B:379:ILE:O	1:B:383:MET:HG3	2.09	0.53
1:A:460:ARG:NE	1:A:506:VAL:HG13	2.23	0.53
2:E:334:PHE:CE2	2:E:386:SER:HB2	2.43	0.53
1:B:237:TYR:CE2	1:B:451:PRO:HG2	2.44	0.53
1:B:215:TYR:HE2	1:B:568:LEU:HD23	1.74	0.53
1:A:144:LEU:HD22	1:A:168:TRP:CZ2	2.44	0.53
1:B:184:VAL:HG12	1:B:188:ASN:HD22	1.72	0.53
1:A:580:ASN:ND2	1:A:582:ARG:H	2.07	0.53
1:A:499:ASP:O	1:A:501:ALA:N	2.42	0.53
2:F:329:PHE:CZ	2:F:497:VAL:HG11	2.43	0.53
1:B:557:MET:HB3	1:B:573:VAL:CG1	2.39	0.53
1:B:166:GLU:HA	1:B:166:GLU:OE1	2.09	0.53
1:A:571:GLU:O	1:A:573:VAL:N	2.42	0.53
2:F:403:GLY:C	2:F:405:ILE:H	2.12	0.53
2:E:409:ASN:HD21	2:E:441:ARG:N	1.99	0.53
1:B:159:ASN:O	1:B:162:LEU:HB3	2.09	0.53
2:F:396:GLN:OE1	2:F:403:GLY:HA2	2.09	0.53
1:B:554:LEU:O	1:B:555:PHE:C	2.46	0.53
1:B:122:THR:HG22	1:B:126:ILE:HD11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:TRP:O	1:B:172:VAL:HG22	2.09	0.52
1:B:290:ASN:HB3	1:B:292:ASP:H	1.73	0.52
1:A:545:SER:O	1:A:547:SER:N	2.41	0.52
1:A:501:ALA:HA	1:A:506:VAL:HB	1.91	0.52
2:E:332:THR:HG23	2:E:333:LYS:HG3	1.89	0.52
1:A:540:HIS:HE1	1:A:590:PRO:HG2	1.74	0.52
1:B:122:THR:O	1:B:126:ILE:HG13	2.10	0.52
1:B:335:ASP:HB2	1:B:361:CYS:HB3	1.90	0.52
1:A:81:GLN:HE21	1:A:81:GLN:CA	2.22	0.52
1:A:88:ILE:HG21	1:A:94:LYS:HB2	1.91	0.52
1:B:455:MET:O	1:B:456:LEU:C	2.47	0.52
2:F:413:PRO:HG2	2:F:416:PHE:O	2.10	0.52
1:A:556:ASN:O	1:A:560:LEU:HG	2.10	0.52
1:A:177:ARG:HB3	1:A:178:PRO:HD3	1.91	0.52
1:A:603:PHE:HD2	1:A:603:PHE:C	2.13	0.52
1:B:252:TYR:CD2	1:B:266:LEU:HD13	2.44	0.52
2:F:403:GLY:O	2:F:404:VAL:HB	2.09	0.52
1:B:204:ARG:HG2	1:B:222:LEU:HD23	1.92	0.52
1:B:320:LEU:HD13	1:B:380:GLN:HG2	1.92	0.52
1:A:379:ILE:O	1:A:383:MET:HG3	2.09	0.52
1:B:309:LYS:HD2	1:B:328:TRP:CH2	2.45	0.52
1:A:177:ARG:O	1:A:181:GLU:HG3	2.10	0.52
2:E:351:ASP:O	2:E:352:TYR:HB2	2.10	0.52
1:A:400:PHE:CE2	1:A:557:MET:HE3	2.45	0.52
2:F:372:THR:HG22	2:F:373:LYS:N	2.25	0.52
1:A:398:GLU:OE1	1:A:514:ARG:HB3	2.10	0.52
1:A:351:LEU:HD12	1:A:351:LEU:H	1.75	0.52
2:E:357:ASN:O	2:E:358:SER:HB3	2.10	0.52
2:F:431:THR:HG23	2:F:435:ASN:HB2	1.92	0.52
1:B:524:GLN:NE2	1:B:580:ASN:H	2.07	0.52
1:B:184:VAL:HG12	1:B:188:ASN:ND2	2.25	0.52
2:E:361:PHE:N	2:E:361:PHE:HD2	2.08	0.52
1:B:199:TYR:O	1:B:202:TYR:HB3	2.10	0.52
1:A:407:ILE:HD11	1:A:522:GLN:O	2.09	0.51
1:A:179:LEU:CD1	1:A:179:LEU:H	2.17	0.51
2:E:406:ALA:HA	2:E:410:TYR:O	2.10	0.51
2:E:416:PHE:CD1	2:E:416:PHE:N	2.78	0.51
2:E:361:PHE:N	2:E:361:PHE:CD2	2.77	0.51
1:A:211:GLY:O	1:A:212:VAL:HG13	2.11	0.51
2:E:388:VAL:CG2	2:E:495:ARG:HG2	2.39	0.51
1:A:213:ASP:O	1:A:215:TYR:HD1	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:ARG:NH2	1:B:260:GLY:O	2.44	0.51
1:B:482:ARG:HE	1:B:488:VAL:HG12	1.76	0.51
1:B:609:ASP:O	1:B:610:TRP:C	2.49	0.51
2:F:383:TYR:HB2	2:F:500:SER:HB2	1.92	0.51
1:B:524:GLN:HA	1:B:583:PRO:HG2	1.91	0.51
1:A:259:ILE:HG13	1:A:259:ILE:O	2.09	0.51
1:A:24:LEU:HD22	2:E:473:ASN:ND2	2.26	0.51
1:B:213:ASP:O	1:B:215:TYR:HD1	1.94	0.51
1:A:603:PHE:CD2	1:A:603:PHE:C	2.82	0.51
1:A:166:GLU:HA	1:A:166:GLU:OE1	2.10	0.51
1:A:279:TYR:CZ	1:A:283:VAL:HG23	2.46	0.51
1:A:339:VAL:O	1:A:339:VAL:HG12	2.11	0.51
2:E:369:VAL:O	2:E:370:SER:HB2	2.10	0.51
1:B:351:LEU:H	1:B:351:LEU:HD12	1.76	0.51
1:B:177:ARG:HB3	1:B:178:PRO:HD3	1.93	0.51
1:B:474:MET:HE1	1:B:499:ASP:HB2	1.91	0.51
1:B:366:MET:CE	1:B:441:LYS:HZ3	2.24	0.51
1:B:271:TRP:CD2	1:B:503:LEU:HD23	2.45	0.51
1:B:259:ILE:HA	1:B:603:PHE:HD1	1.76	0.51
2:E:449:ARG:O	2:E:452:GLU:HB2	2.10	0.51
1:A:154:ASN:O	1:A:156:LEU:HD22	2.11	0.51
1:B:179:LEU:HD12	1:B:179:LEU:N	2.16	0.50
1:B:487:VAL:HG12	1:B:488:VAL:H	1.76	0.50
1:B:353:LYS:HB3	2:F:487:THR:CG2	2.41	0.50
1:A:335:ASP:HB2	1:A:361:CYS:HB3	1.93	0.50
1:A:499:ASP:C	1:A:501:ALA:N	2.65	0.50
1:B:480:MET:C	1:B:482:ARG:H	2.14	0.50
2:E:423:TRP:NE1	2:E:495:ARG:HB2	2.26	0.50
1:A:352:GLY:O	1:A:353:LYS:HB2	2.10	0.50
2:F:417:MET:HA	2:F:417:MET:CE	2.41	0.50
1:B:456:LEU:HD21	1:B:460:ARG:HD2	1.94	0.50
1:A:402:GLU:HB3	1:A:518:ARG:HD2	1.93	0.50
1:B:407:ILE:HD11	1:B:522:GLN:O	2.12	0.50
1:B:474:MET:CE	1:B:499:ASP:H	2.25	0.50
2:E:432:SER:HA	2:E:485:THR:HG22	1.92	0.50
1:B:177:ARG:NH2	1:B:495:GLU:O	2.44	0.50
1:B:30:GLU:O	1:B:34:TYR:CD1	2.60	0.50
2:F:412:LEU:HD21	2:F:417:MET:SD	2.52	0.50
1:B:448:GLY:O	1:B:451:PRO:HD2	2.12	0.50
1:A:503:LEU:O	1:A:504:PHE:C	2.50	0.50
1:B:81:GLN:NE2	1:B:101:GLN:HE22	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:ILE:O	1:B:291:ILE:HG22	2.11	0.50
2:E:469:PRO:HG3	2:E:476:TRP:NE1	2.27	0.50
1:B:115:ARG:O	1:B:119:ILE:HG12	2.11	0.50
1:B:97:LEU:O	1:B:101:GLN:HG2	2.12	0.49
1:B:526:GLN:HG3	1:B:539:LEU:HD11	1.93	0.49
1:B:75:GLU:O	1:B:79:LEU:HB2	2.11	0.49
1:B:180:TYR:HA	1:B:183:TYR:HB3	1.94	0.49
1:B:207:TYR:CE1	1:B:398:GLU:OE2	2.66	0.49
1:A:397:ASN:OD1	1:A:399:GLY:N	2.37	0.49
1:A:581:VAL:CG2	1:A:584:LEU:HD23	2.42	0.49
1:B:270:MET:HB3	1:B:271:TRP:CE3	2.46	0.49
1:A:223:ILE:O	1:A:227:GLU:HG3	2.11	0.49
1:A:543:ASP:C	1:A:545:SER:H	2.16	0.49
1:B:134:ASN:HB3	1:B:137:ASN:HB3	1.93	0.49
2:E:483:PHE:HB3	2:E:493:PRO:HD3	1.93	0.49
1:A:529:LEU:HB3	1:A:544:ILE:CG2	2.43	0.49
1:A:455:MET:HE2	1:A:485:VAL:HG21	1.94	0.49
1:A:215:TYR:CD2	1:A:568:LEU:HB2	2.47	0.49
1:A:119:ILE:O	1:A:120:LEU:C	2.51	0.49
2:F:345:ILE:O	2:F:382:VAL:HG12	2.12	0.49
1:B:395:GLY:O	1:B:396:ALA:C	2.50	0.49
1:A:507:SER:C	1:A:508:ASN:HD22	2.16	0.49
1:B:81:GLN:HE22	1:B:101:GLN:HE22	1.61	0.49
1:A:24:LEU:HD22	2:E:473:ASN:HD22	1.76	0.49
1:B:289:PRO:C	1:B:290:ASN:O	2.51	0.49
1:A:279:TYR:CE1	1:A:441:LYS:HB2	2.48	0.49
1:A:279:TYR:O	1:A:280:SER:C	2.51	0.49
1:A:239:HIS:CE1	1:A:604:VAL:HG21	2.48	0.49
2:E:423:TRP:HE1	2:E:495:ARG:HB2	1.77	0.49
2:E:453:ARG:CZ	2:E:455:ILE:HD11	2.43	0.49
1:A:323:MET:CE	1:A:323:MET:HA	2.43	0.49
1:A:404:VAL:O	1:A:407:ILE:HB	2.12	0.49
2:F:423:TRP:HE1	2:F:495:ARG:HB2	1.78	0.49
1:B:366:MET:O	1:B:369:PHE:N	2.45	0.49
2:E:459:PRO:HB2	2:E:467:CYS:CB	2.43	0.49
2:F:362:SER:O	2:F:363:THR:OG1	2.30	0.49
1:B:56:GLU:HA	1:B:59:VAL:HG12	1.95	0.48
1:A:251:ALA:C	1:A:253:PRO:HD3	2.34	0.48
1:B:525:PHE:O	1:B:529:LEU:HB2	2.12	0.48
1:A:555:PHE:O	1:A:559:ARG:HG2	2.12	0.48
1:A:289:PRO:C	1:A:290:ASN:HD22	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:GLU:O	1:A:79:LEU:HB2	2.13	0.48
1:A:270:MET:HB3	1:A:271:TRP:CZ3	2.49	0.48
1:A:41:TYR:O	1:A:45:VAL:HG23	2.14	0.48
2:F:361:PHE:N	2:F:361:PHE:CD2	2.81	0.48
2:F:459:PRO:HB2	2:F:467:CYS:HB2	1.95	0.48
1:A:46:ALA:HB1	1:A:62:MET:HA	1.96	0.48
1:B:476:LYS:O	1:B:480:MET:HG3	2.14	0.48
1:B:237:TYR:CZ	1:B:451:PRO:HG2	2.49	0.48
1:B:499:ASP:O	1:B:502:SER:N	2.39	0.48
2:F:388:VAL:HG22	2:F:495:ARG:HA	1.94	0.48
1:A:557:MET:SD	1:A:558:LEU:CD1	3.01	0.48
1:B:107:VAL:HG21	1:B:193:ALA:CB	2.42	0.48
1:A:49:ASN:HB3	1:A:58:ASN:HD22	1.79	0.48
1:B:211:GLY:N	1:B:216:ASP:OD2	2.46	0.48
1:B:261:CYS:CB	1:B:488:VAL:HG13	2.44	0.48
1:B:291:ILE:O	1:B:366:MET:SD	2.71	0.48
1:A:320:LEU:HD13	1:A:380:GLN:HG2	1.96	0.48
2:F:367:TYR:CD1	2:F:367:TYR:N	2.82	0.48
1:A:52:THR:HG22	1:A:359:LEU:HD13	1.94	0.48
1:A:363:LYS:O	1:A:365:THR:N	2.47	0.48
2:F:396:GLN:OE1	2:F:405:ILE:HB	2.14	0.48
1:A:594:TRP:O	1:A:598:GLN:HG2	2.14	0.48
2:E:453:ARG:NH1	2:E:455:ILE:HD11	2.29	0.48
1:A:158:TYR:CE1	1:A:265:HIS:NE2	2.80	0.48
1:B:369:PHE:CD1	1:B:370:LEU:HD23	2.49	0.48
1:A:99:ALA:O	1:A:102:GLN:HG3	2.13	0.48
2:E:367:TYR:N	2:E:367:TYR:CD1	2.82	0.48
1:A:485:VAL:O	1:A:485:VAL:HG12	2.13	0.47
1:B:581:VAL:HG22	1:B:585:LEU:HD23	1.96	0.47
1:B:611:SER:HB2	1:B:614:ALA:HB3	1.95	0.47
1:A:262:LEU:O	1:A:487:VAL:HG13	2.13	0.47
1:B:456:LEU:HD22	1:B:512:PHE:CD1	2.49	0.47
2:E:329:PHE:C	2:E:331:ALA:N	2.68	0.47
1:B:450:LEU:HA	1:B:450:LEU:HD12	1.69	0.47
1:A:180:TYR:HA	1:A:183:TYR:HB3	1.96	0.47
1:A:180:TYR:O	1:A:183:TYR:HB3	2.15	0.47
1:B:557:MET:HB3	1:B:573:VAL:HG11	1.96	0.47
1:A:499:ASP:N	1:A:500:PRO:HD2	2.29	0.47
1:B:512:PHE:C	1:B:514:ARG:H	2.17	0.47
1:B:84:PRO:HG2	1:B:87:GLU:OE1	2.14	0.47
1:B:410:LEU:HD21	1:B:523:PHE:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:589:GLU:OE1	1:B:589:GLU:HA	2.12	0.47
1:A:82:THR:HB	1:A:83:TYR:CE1	2.49	0.47
1:A:102:GLN:C	1:A:104:GLY:N	2.67	0.47
1:A:440:LEU:C	1:A:442:GLN:N	2.67	0.47
1:B:548:THR:O	1:B:552:GLN:N	2.47	0.47
1:A:452:PHE:CE2	1:A:481:LYS:NZ	2.82	0.47
2:E:361:PHE:HE1	2:E:421:LEU:HD23	1.79	0.47
1:B:274:PHE:CD2	1:B:449:THR:HB	2.50	0.47
1:B:194:ASN:O	1:B:195:HIS:HB2	2.14	0.47
2:F:344:LYS:HE3	2:F:346:SER:OG	2.14	0.47
1:B:262:LEU:O	1:B:487:VAL:HG13	2.14	0.47
1:A:137:ASN:H	1:A:138:PRO:HD3	1.79	0.47
1:B:521:TYR:O	1:B:522:GLN:C	2.52	0.47
1:A:554:LEU:O	1:A:556:ASN:N	2.48	0.47
1:B:41:TYR:O	1:B:45:VAL:HG23	2.14	0.47
1:B:273:ARG:HG2	1:B:273:ARG:HH21	1.79	0.47
1:B:414:THR:O	1:B:418:LEU:CD2	2.62	0.47
2:F:452:GLU:CG	2:F:453:ARG:H	2.25	0.47
1:A:456:LEU:CD1	1:A:460:ARG:HD2	2.45	0.47
1:B:549:GLU:N	1:B:549:GLU:CD	2.65	0.47
1:A:288:LYS:HD2	1:A:434:THR:CG2	2.45	0.47
1:B:339:VAL:O	1:B:339:VAL:HG12	2.15	0.47
1:B:157:ASP:HB3	1:B:160:GLU:HB3	1.96	0.47
1:B:302:TRP:CZ2	1:B:423:LEU:HD21	2.50	0.47
1:B:211:GLY:C	1:B:212:VAL:HG22	2.35	0.47
1:B:564:GLU:HB3	1:B:568:LEU:HD12	1.97	0.47
1:B:456:LEU:C	1:B:456:LEU:HD23	2.35	0.47
1:B:257:SER:HB3	1:B:260:GLY:HA3	1.97	0.47
1:B:586:ASN:O	1:B:588:PHE:N	2.48	0.47
1:A:85:LEU:O	1:A:88:ILE:HD13	2.15	0.46
1:B:94:LYS:O	1:B:98:GLN:HB2	2.16	0.46
1:A:454:TYR:HD1	1:A:484:ILE:HG21	1.79	0.46
1:B:389:PRO:CG	1:B:392:LEU:HD22	2.46	0.46
1:A:407:ILE:CD1	1:A:526:GLN:HG2	2.46	0.46
1:A:305:GLN:O	1:A:309:LYS:HB2	2.15	0.46
2:F:449:ARG:O	2:F:452:GLU:HB2	2.14	0.46
1:B:209:VAL:HB	1:B:216:ASP:CA	2.35	0.46
2:E:397:ILE:O	2:E:420:VAL:HG21	2.15	0.46
1:B:389:PRO:HG2	1:B:392:LEU:HD22	1.95	0.46
1:A:103:ASN:HD21	1:A:107:VAL:HB	1.80	0.46
1:B:46:ALA:HB1	1:B:62:MET:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:512:PHE:C	1:B:514:ARG:N	2.69	0.46
2:F:335:PRO:HG2	2:F:387:PHE:HA	1.97	0.46
1:B:170:SER:O	1:B:174:LYS:HG3	2.15	0.46
1:B:144:LEU:HB2	1:B:168:TRP:CH2	2.50	0.46
1:A:259:ILE:HB	1:A:603:PHE:CD1	2.50	0.46
1:B:375:GLU:OE1	1:B:378:HIS:HD2	1.98	0.46
1:B:251:ALA:HB1	1:B:281:LEU:HD22	1.97	0.46
1:A:407:ILE:HD12	1:A:526:GLN:HG2	1.96	0.46
1:A:437:ASN:O	1:A:438:PHE:C	2.54	0.46
2:F:361:PHE:HE1	2:F:421:LEU:HD23	1.81	0.46
1:B:381:TYR:CG	1:B:558:LEU:HD22	2.50	0.46
1:A:466:GLY:C	1:A:468:ILE:H	2.19	0.46
1:B:251:ALA:C	1:B:253:PRO:HD3	2.36	0.46
1:A:93:VAL:O	1:A:97:LEU:HB2	2.16	0.46
2:E:412:LEU:HD21	2:E:417:MET:SD	2.55	0.46
1:B:474:MET:HE2	1:B:499:ASP:H	1.79	0.46
1:A:229:THR:OG1	1:A:581:VAL:HB	2.16	0.46
1:B:586:ASN:C	1:B:588:PHE:N	2.68	0.46
1:A:504:PHE:C	1:A:504:PHE:CD2	2.90	0.46
1:A:175:GLN:O	1:A:179:LEU:CD1	2.64	0.46
1:B:81:GLN:C	1:B:83:TYR:H	2.19	0.46
1:B:291:ILE:HG21	1:B:438:PHE:HD1	1.80	0.46
1:A:274:PHE:CE2	1:A:449:THR:CB	2.99	0.45
1:A:540:HIS:CE1	1:A:590:PRO:HG2	2.51	0.45
1:B:553:LYS:HE3	1:B:573:VAL:HA	1.98	0.45
1:B:305:GLN:O	1:B:309:LYS:HB2	2.16	0.45
1:A:291:ILE:O	1:A:366:MET:SD	2.74	0.45
1:B:177:ARG:CZ	1:B:473:TRP:HE3	2.29	0.45
1:B:396:ALA:HB1	1:B:566:TRP:HA	1.97	0.45
1:A:274:PHE:CE2	1:A:449:THR:HB	2.51	0.45
1:B:123:MET:HE1	1:B:183:TYR:HB2	1.97	0.45
1:A:223:ILE:H	1:A:223:ILE:HG13	1.57	0.45
2:F:365:LYS:HB3	2:F:367:TYR:CE1	2.51	0.45
1:B:135:PRO:CD	1:B:163:TRP:HE1	2.29	0.45
2:F:483:PHE:HB3	2:F:493:PRO:HD3	1.98	0.45
2:E:340:TRP:CE3	2:E:385:ASP:HB3	2.51	0.45
1:B:49:ASN:HB3	1:B:58:ASN:HD22	1.82	0.45
1:A:460:ARG:HH12	1:A:512:PHE:HB2	1.81	0.45
1:B:269:ASP:OD2	1:B:269:ASP:C	2.54	0.45
1:A:167:SER:O	1:A:171:GLU:HG2	2.15	0.45
2:F:372:THR:HG22	2:F:373:LYS:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:589:GLU:H	1:A:590:PRO:HD3	1.80	0.45
1:B:389:PRO:O	1:B:391:LEU:N	2.49	0.45
1:A:285:PHE:HE1	1:A:436:ILE:HG21	1.80	0.45
1:B:100:LEU:C	1:B:102:GLN:H	2.20	0.45
2:F:485:THR:HG23	2:F:486:THR:HG23	1.99	0.45
1:A:543:ASP:C	1:A:545:SER:N	2.68	0.45
1:B:358:ILE:HD13	1:B:375:GLU:HB3	1.98	0.45
1:B:88:ILE:HG21	1:B:94:LYS:HB2	1.97	0.45
1:B:273:ARG:HG2	1:B:273:ARG:NH2	2.32	0.45
2:E:338:TYR:CE1	2:E:339:ALA:HB2	2.52	0.45
1:A:579:MET:O	1:A:579:MET:CG	2.65	0.45
1:A:123:MET:HE1	1:A:183:TYR:HB2	1.98	0.45
2:E:386:SER:HA	2:E:496:VAL:O	2.17	0.45
1:A:349:TRP:HB2	1:A:357:ARG:O	2.16	0.45
2:E:431:THR:HG23	2:E:435:ASN:HB2	1.99	0.45
1:B:315:PHE:CZ	1:B:408:MET:HG3	2.51	0.45
1:A:94:LYS:O	1:A:98:GLN:HB2	2.17	0.45
1:A:446:ILE:N	1:A:446:ILE:HD12	2.31	0.45
1:A:439:LEU:HA	1:A:439:LEU:HD22	1.62	0.45
1:B:241:HIS:O	1:B:244:VAL:HG22	2.17	0.45
2:F:361:PHE:HD2	2:F:361:PHE:N	2.14	0.45
1:A:35:GLU:OE1	2:E:479:ARG:NH1	2.50	0.45
1:B:192:ARG:HH21	1:B:192:ARG:HG2	1.81	0.45
1:A:208:GLU:HB2	1:A:219:ARG:HG2	1.98	0.45
1:A:450:LEU:CB	1:A:451:PRO:HD3	2.47	0.45
1:B:584:LEU:C	1:B:584:LEU:HD23	2.38	0.45
1:A:320:LEU:HD13	1:A:380:GLN:CG	2.47	0.44
1:B:316:VAL:O	1:B:318:VAL:N	2.51	0.44
1:B:256:ILE:HG22	1:B:257:SER:N	2.32	0.44
1:A:323:MET:HA	1:A:323:MET:HE2	1.99	0.44
1:B:467:GLU:O	1:B:469:PRO:HD3	2.17	0.44
1:A:407:ILE:HA	1:A:407:ILE:HD13	1.67	0.44
1:B:541:LYS:HA	1:B:541:LYS:CE	2.47	0.44
1:B:554:LEU:O	1:B:556:ASN:N	2.51	0.44
1:B:373:HIS:CD2	1:B:412:ALA:HB2	2.52	0.44
1:A:274:PHE:HE2	1:A:449:THR:HG21	1.82	0.44
1:A:591:LEU:O	1:A:592:PHE:C	2.54	0.44
1:A:122:THR:O	1:A:126:ILE:HG13	2.17	0.44
1:B:303:ASP:O	1:B:304:ALA:C	2.56	0.44
1:A:529:LEU:HB3	1:A:544:ILE:HG21	1.98	0.44
1:B:213:ASP:O	1:B:215:TYR:CD1	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:GLN:NE2	1:A:101:GLN:HE22	2.15	0.44
1:A:400:PHE:CD2	1:A:557:MET:CE	2.97	0.44
1:B:512:PHE:O	1:B:514:ARG:N	2.51	0.44
2:E:459:PRO:CB	2:E:467:CYS:CB	2.96	0.44
1:A:417:HIS:O	1:A:420:SER:HB3	2.18	0.44
1:B:455:MET:O	1:B:458:LYS:N	2.51	0.44
1:B:455:MET:HE1	1:B:456:LEU:HA	2.00	0.44
1:A:284:PRO:HB3	1:A:594:TRP:CH2	2.53	0.44
1:B:101:GLN:HA	1:B:101:GLN:HE21	1.83	0.44
1:B:81:GLN:C	1:B:83:TYR:N	2.71	0.44
1:A:30:GLU:O	1:A:34:TYR:CD1	2.66	0.44
2:F:359:THR:O	2:F:361:PHE:N	2.51	0.44
1:A:410:LEU:HA	1:A:410:LEU:HD12	1.86	0.44
1:B:363:LYS:N	1:B:368:ASP:OD2	2.51	0.44
2:F:405:ILE:HG22	2:F:406:ALA:N	2.33	0.44
1:A:474:MET:HE1	1:A:499:ASP:H	1.81	0.43
1:B:483:GLU:HA	1:B:606:TRP:HE1	1.83	0.43
2:F:329:PHE:C	2:F:331:ALA:N	2.72	0.43
1:A:557:MET:C	1:A:557:MET:SD	2.97	0.43
1:B:251:ALA:HB2	1:B:281:LEU:HD22	2.00	0.43
1:A:514:ARG:HG3	1:A:515:TYR:N	2.32	0.43
1:A:394:ASN:O	1:A:561:GLY:HA2	2.17	0.43
1:A:56:GLU:HA	1:A:59:VAL:HG12	2.00	0.43
1:A:143:LEU:O	1:A:146:PRO:O	2.36	0.43
2:F:409:ASN:HD21	2:F:441:ARG:N	2.15	0.43
1:A:249:MET:HG2	1:A:256:ILE:HB	2.00	0.43
2:F:369:VAL:HB	2:F:370:SER:H	1.52	0.43
1:B:599:ASN:O	1:B:602:SER:N	2.38	0.43
1:A:568:LEU:O	1:A:571:GLU:HB3	2.17	0.43
1:B:188:ASN:O	1:B:192:ARG:HG3	2.18	0.43
2:E:449:ARG:O	2:E:450:PRO:C	2.57	0.43
1:A:84:PRO:HG2	1:A:87:GLU:OE1	2.17	0.43
1:B:252:TYR:HD2	1:B:266:LEU:HD13	1.83	0.43
1:A:591:LEU:O	1:A:594:TRP:N	2.51	0.43
1:B:535:HIS:CE1	1:B:542:CYS:HA	2.53	0.43
1:A:494:ASP:OD1	1:A:496:THR:HG22	2.19	0.43
2:F:469:PRO:HG3	2:F:476:TRP:CZ2	2.54	0.43
1:A:524:GLN:HG2	1:A:524:GLN:H	1.52	0.43
1:A:77:SER:C	1:A:79:LEU:N	2.72	0.43
1:B:119:ILE:O	1:B:120:LEU:C	2.56	0.43
2:F:367:TYR:HD1	2:F:367:TYR:H	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:478:TRP:C	1:B:480:MET:N	2.70	0.43
1:B:249:MET:HE3	1:B:258:PRO:HG3	2.00	0.43
1:B:320:LEU:HD13	1:B:380:GLN:CG	2.48	0.43
2:F:415:ASP:O	2:F:416:PHE:C	2.56	0.43
1:B:407:ILE:HA	1:B:407:ILE:HD13	1.58	0.43
1:B:599:ASN:O	1:B:601:ASN:N	2.51	0.43
1:B:186:LEU:O	1:B:189:GLU:HB2	2.18	0.43
1:B:582:ARG:HA	1:B:582:ARG:NE	2.32	0.43
1:A:101:GLN:NE2	1:A:101:GLN:HA	2.34	0.43
1:A:545:SER:C	1:A:547:SER:H	2.22	0.43
1:A:581:VAL:HG23	1:A:584:LEU:HD23	2.00	0.43
1:B:607:SER:C	1:B:609:ASP:H	2.22	0.43
2:F:432:SER:HA	2:F:485:THR:HG22	2.00	0.43
1:B:279:TYR:O	1:B:280:SER:C	2.57	0.43
1:B:144:LEU:HD22	1:B:168:TRP:CZ2	2.53	0.43
1:B:302:TRP:CE2	1:B:423:LEU:HD21	2.53	0.43
1:A:439:LEU:O	1:A:442:GLN:HB2	2.19	0.43
1:A:582:ARG:HB3	1:A:583:PRO:HD3	2.01	0.43
1:B:494:ASP:OD1	1:B:496:THR:OG1	2.30	0.43
1:B:176:LEU:HA	1:B:179:LEU:HD13	2.00	0.42
1:B:530:CYS:O	1:B:533:ALA:N	2.52	0.42
1:B:249:MET:CE	1:B:258:PRO:HG3	2.49	0.42
1:B:208:GLU:HB2	1:B:219:ARG:HG2	2.01	0.42
1:B:248:LEU:O	1:B:251:ALA:N	2.53	0.42
1:B:274:PHE:CE2	1:B:449:THR:HB	2.54	0.42
1:A:53:ASN:O	1:A:54:ILE:C	2.57	0.42
1:A:599:ASN:N	1:A:599:ASN:HD22	2.16	0.42
1:B:465:LYS:HB3	1:B:465:LYS:HE2	1.84	0.42
1:A:74:LYS:NZ	1:A:78:THR:HG21	2.35	0.42
1:B:480:MET:C	1:B:482:ARG:N	2.72	0.42
1:B:381:TYR:CE2	1:B:558:LEU:O	2.69	0.42
2:F:332:THR:HG23	2:F:333:LYS:H	1.84	0.42
1:B:580:ASN:C	1:B:582:ARG:N	2.72	0.42
1:B:171:GLU:HB2	1:B:172:VAL:H	1.62	0.42
1:A:396:ALA:HB3	1:A:400:PHE:CG	2.54	0.42
1:A:137:ASN:N	1:A:138:PRO:HD3	2.33	0.42
1:B:466:GLY:O	1:B:467:GLU:C	2.58	0.42
1:A:53:ASN:O	1:A:55:THR:HG23	2.19	0.42
1:A:162:LEU:HD13	1:A:490:PRO:HB2	2.01	0.42
1:B:477:TRP:HD1	1:B:478:TRP:CD1	2.38	0.42
1:B:491:VAL:HA	1:B:613:TYR:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:GLU:O	1:B:59:VAL:HG12	2.19	0.42
1:A:555:PHE:CD1	1:A:555:PHE:O	2.73	0.42
1:B:599:ASN:O	1:B:600:LYS:C	2.57	0.42
1:A:177:ARG:HH22	1:A:495:GLU:HA	1.85	0.42
2:F:369:VAL:O	2:F:370:SER:HB2	2.20	0.42
2:E:413:PRO:HB2	2:E:416:PHE:HD1	1.84	0.42
1:A:475:LYS:O	1:A:479:GLU:HB2	2.18	0.42
1:B:77:SER:C	1:B:79:LEU:N	2.73	0.42
2:F:351:ASP:O	2:F:352:TYR:CB	2.67	0.42
1:B:451:PRO:O	1:B:452:PHE:C	2.58	0.42
2:E:367:TYR:H	2:E:367:TYR:HD1	1.67	0.42
1:A:517:THR:HB	1:A:521:TYR:CE2	2.55	0.42
1:A:485:VAL:HG12	1:A:487:VAL:CG2	2.50	0.42
2:F:390:LYS:HB3	2:F:393:ASP:HB2	2.01	0.42
1:B:538:PRO:HB3	1:B:540:HIS:CE1	2.54	0.42
1:A:269:ASP:OD2	1:A:269:ASP:C	2.58	0.42
1:B:463:VAL:HG13	1:B:473:TRP:NE1	2.32	0.42
1:B:463:VAL:CG1	1:B:473:TRP:HE1	2.30	0.42
2:E:417:MET:CE	2:E:417:MET:HA	2.50	0.42
1:B:209:VAL:HG11	1:B:215:TYR:O	2.20	0.42
1:A:520:LEU:HD22	1:A:520:LEU:N	2.26	0.42
1:A:288:LYS:HD2	1:A:434:THR:HG23	2.02	0.42
2:F:469:PRO:HA	2:F:471:ALA:H	1.85	0.42
1:A:85:LEU:CD1	1:A:85:LEU:H	2.26	0.41
2:F:423:TRP:NE1	2:F:495:ARG:HB2	2.35	0.41
1:A:442:GLN:O	1:A:443:ALA:C	2.57	0.41
1:A:467:GLU:C	1:A:468:ILE:HG13	2.40	0.41
1:A:59:VAL:HG13	1:A:60:GLN:N	2.34	0.41
1:A:535:HIS:CE1	1:A:542:CYS:HA	2.55	0.41
1:A:229:THR:HG23	1:A:230:PHE:N	2.35	0.41
1:B:588:PHE:O	1:B:591:LEU:N	2.53	0.41
1:A:125:THR:HA	1:A:128:SER:OG	2.20	0.41
1:B:57:GLU:O	1:B:61:ASN:HB2	2.20	0.41
1:A:89:GLN:O	1:A:91:LEU:N	2.52	0.41
1:A:88:ILE:CG2	1:A:94:LYS:HB2	2.50	0.41
1:B:402:GLU:HB3	1:B:518:ARG:CD	2.50	0.41
1:B:457:GLU:O	1:B:461:TRP:HB2	2.20	0.41
1:B:187:LYS:HE3	1:B:509:ASP:OD2	2.21	0.41
2:E:359:THR:O	2:E:361:PHE:N	2.53	0.41
1:A:402:GLU:HB3	1:A:518:ARG:HD3	2.02	0.41
1:B:353:LYS:HB3	2:F:487:THR:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:TYR:CZ	1:B:283:VAL:HG23	2.55	0.41
1:A:415:PRO:O	1:A:419:LYS:HG3	2.19	0.41
1:B:582:ARG:CB	1:B:583:PRO:HD3	2.33	0.41
1:B:72:PHE:CE2	1:B:76:GLN:HG3	2.55	0.41
1:A:237:TYR:O	1:A:238:GLU:C	2.57	0.41
2:E:337:VAL:HG22	2:E:388:VAL:O	2.20	0.41
1:B:137:ASN:N	1:B:138:PRO:HD3	2.33	0.41
1:B:316:VAL:C	1:B:318:VAL:N	2.73	0.41
1:B:169:ARG:HH12	1:B:271:TRP:HA	1.85	0.41
1:B:366:MET:HE1	1:B:441:LYS:HZ3	1.85	0.41
1:B:183:TYR:O	1:B:187:LYS:HB2	2.20	0.41
1:A:201:ASP:OD2	1:A:219:ARG:NH2	2.53	0.41
1:B:414:THR:O	1:B:418:LEU:HD22	2.21	0.41
2:F:469:PRO:HG3	2:F:476:TRP:NE1	2.36	0.41
2:F:337:VAL:O	2:F:340:TRP:HD1	2.04	0.41
2:E:372:THR:HG22	2:E:374:LEU:HD12	2.03	0.41
1:B:177:ARG:NE	1:B:473:TRP:CE3	2.88	0.41
1:B:499:ASP:O	1:B:500:PRO:C	2.57	0.41
1:B:323:MET:HA	1:B:323:MET:CE	2.51	0.41
1:A:546:ASN:HD22	1:A:546:ASN:HA	1.74	0.41
2:E:364:PHE:O	2:E:365:LYS:C	2.59	0.41
1:B:568:LEU:HD13	1:B:572:ASN:HD21	1.86	0.41
2:F:423:TRP:CD1	2:F:423:TRP:N	2.87	0.41
1:B:456:LEU:CD2	1:B:460:ARG:HD2	2.51	0.41
2:E:332:THR:HG23	2:E:333:LYS:HE3	2.02	0.41
1:B:504:PHE:C	1:B:504:PHE:CD2	2.94	0.41
1:A:580:ASN:HD21	1:A:582:ARG:HB2	1.85	0.41
1:A:335:ASP:HA	1:A:336:PRO:HD3	1.93	0.41
1:B:414:THR:O	1:B:418:LEU:HD23	2.21	0.41
1:A:366:MET:O	1:A:369:PHE:N	2.54	0.41
1:A:228:HIS:O	1:A:231:GLU:HB2	2.20	0.41
1:A:166:GLU:OE2	1:A:493:HIS:HE1	2.04	0.41
1:A:517:THR:HA	1:A:520:LEU:HD23	2.03	0.41
1:A:581:VAL:O	1:A:581:VAL:HG22	2.19	0.41
1:B:223:ILE:H	1:B:223:ILE:HG13	1.63	0.41
1:B:312:GLU:O	1:B:316:VAL:HG23	2.21	0.41
1:B:504:PHE:O	1:B:506:VAL:N	2.53	0.41
1:B:352:GLY:O	1:B:353:LYS:HB2	2.21	0.41
1:B:410:LEU:HA	1:B:410:LEU:HD12	1.89	0.41
1:A:291:ILE:O	1:A:291:ILE:HG22	2.20	0.41
2:E:442:TYR:CD1	2:E:443:LEU:HG	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:HIS:CE1	1:B:596:LYS:HA	2.56	0.41
1:A:110:GLU:O	1:A:114:LYS:HB2	2.21	0.41
1:A:500:PRO:O	1:A:506:VAL:HG11	2.21	0.41
1:B:582:ARG:CB	1:B:583:PRO:CD	2.97	0.41
1:A:544:ILE:O	1:A:545:SER:O	2.39	0.41
2:E:361:PHE:CE1	2:E:421:LEU:HD23	2.55	0.41
1:A:47:SER:HA	1:A:62:MET:HG3	2.03	0.41
1:B:304:ALA:O	1:B:307:ILE:N	2.54	0.41
1:B:262:LEU:HA	1:B:263:PRO:HD3	1.79	0.40
1:A:229:THR:HG23	1:A:516:TYR:OH	2.21	0.40
1:B:79:LEU:C	1:B:81:GLN:H	2.24	0.40
1:B:403:ALA:N	1:B:518:ARG:HG3	2.36	0.40
1:A:591:LEU:HG	1:A:595:LEU:CD1	2.51	0.40
1:B:336:PRO:HB3	1:B:340:GLN:OE1	2.21	0.40
1:A:599:ASN:ND2	1:A:599:ASN:N	2.70	0.40
1:A:181:GLU:OE1	1:A:470:LYS:HE3	2.22	0.40
2:F:357:ASN:O	2:F:358:SER:CB	2.69	0.40
2:E:469:PRO:HG3	2:E:476:TRP:HE1	1.86	0.40
1:B:588:PHE:O	1:B:589:GLU:C	2.60	0.40
2:F:442:TYR:CE2	2:F:479:ARG:HD3	2.57	0.40
1:B:580:ASN:O	1:B:582:ARG:N	2.54	0.40
1:B:290:ASN:C	1:B:292:ASP:H	2.24	0.40
1:A:83:TYR:HA	1:A:84:PRO:HD2	1.95	0.40
1:B:404:VAL:O	1:B:407:ILE:HB	2.22	0.40
1:B:586:ASN:O	1:B:587:TYR:C	2.59	0.40
1:A:231:GLU:OE2	1:A:234:LYS:HE3	2.22	0.40
1:A:63:ASN:O	1:A:67:ASP:N	2.35	0.40
1:B:568:LEU:O	1:B:569:ALA:C	2.59	0.40
1:A:87:GLU:C	1:A:88:ILE:HD12	2.42	0.40
2:F:453:ARG:NH1	2:F:455:ILE:HD11	2.36	0.40
2:E:329:PHE:CE2	2:E:497:VAL:HG11	2.56	0.40
1:A:251:ALA:CB	1:A:281:LEU:HD22	2.51	0.40
1:A:580:ASN:OD1	1:A:583:PRO:HD3	2.21	0.40
1:B:424:LEU:O	1:B:425:SER:C	2.60	0.40
1:A:187:LYS:HE3	1:A:509:ASP:OD2	2.22	0.40
2:F:452:GLU:CG	2:F:453:ARG:N	2.84	0.40
1:A:270:MET:HB3	1:A:271:TRP:CE3	2.56	0.40
2:E:364:PHE:HD1	2:E:364:PHE:O	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	595/603 (99%)	452 (76%)	105 (18%)	38 (6%)	2	9
1	B	595/603 (99%)	444 (75%)	112 (19%)	39 (7%)	1	8
2	E	169/185 (91%)	125 (74%)	29 (17%)	15 (9%)	1	4
2	F	169/185 (91%)	119 (70%)	33 (20%)	17 (10%)	1	3
All	All	1528/1576 (97%)	1140 (75%)	279 (18%)	109 (7%)	1	7

All (109) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	ILE
1	A	137	ASN
1	A	212	VAL
1	A	289	PRO
1	A	340	GLN
1	A	362	THR
1	A	364	VAL
1	A	390	PHE
1	A	544	ILE
1	A	545	SER
1	A	546	ASN
1	A	572	ASN
1	B	54	ILE
1	B	137	ASN
1	B	212	VAL
1	B	290	ASN
1	B	340	GLN
1	B	364	VAL
1	B	390	PHE
1	B	467	GLU
2	E	337	VAL
2	E	360	PHE

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Mol	Chain	Res	Type
2	E	369	VAL
2	E	370	SER
2	E	373	LYS
2	E	404	VAL
2	F	337	VAL
2	F	360	PHE
2	F	369	VAL
2	F	370	SER
2	F	390	LYS
2	F	402	THR
2	F	404	VAL
2	F	416	PHE
1	A	91	LEU
1	A	185	VAL
1	A	211	GLY
1	A	437	ASN
1	A	467	GLU
1	A	509	ASP
1	A	555	PHE
1	A	592	PHE
1	B	86	GLN
1	B	104	GLY
1	B	184	VAL
1	B	185	VAL
1	B	211	GLY
1	B	213	ASP
1	B	268	GLY
1	B	362	THR
1	B	473	TRP
1	B	475	LYS
1	B	504	PHE
1	B	505	HIS
1	B	536	GLU
2	E	330	ASN
2	E	390	LYS
2	E	450	PRO
2	F	373	LYS
1	A	51	ASN
1	A	78	THR
1	A	103	ASN
1	A	268	GLY
1	A	477	TRP

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Mol	Chain	Res	Type
1	A	534	LYS
1	A	539	LEU
1	B	78	THR
1	B	522	GLN
1	B	546	ASN
1	B	610	TRP
2	E	368	GLY
2	E	374	LEU
2	E	401	GLN
2	E	402	THR
2	E	416	PHE
2	F	330	ASN
2	F	374	LEU
2	F	401	GLN
2	F	451	PHE
1	A	206	ASP
1	A	456	LEU
1	A	504	PHE
1	A	571	GLU
1	B	51	ASN
1	B	91	LEU
1	B	171	GLU
1	B	509	ASP
1	B	538	PRO
1	B	581	VAL
1	B	600	LYS
2	F	368	GLY
1	A	104	GLY
1	A	213	ASP
1	B	317	SER
1	B	540	HIS
1	B	587	TYR
2	E	451	PHE
2	F	358	SER
2	F	365	LYS
2	F	450	PRO
1	A	86	GLN
1	A	184	VAL
1	B	20	THR
1	A	500	PRO
1	B	289	PRO
1	A	339	VAL

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Mol	Chain	Res	Type
1	B	451	PRO
1	B	146	PRO
1	A	146	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	527/533 (99%)	483 (92%)	44 (8%)	14	46
1	B	527/533 (99%)	483 (92%)	44 (8%)	14	46
2	E	150/162 (93%)	136 (91%)	14 (9%)	11	39
2	F	150/162 (93%)	134 (89%)	16 (11%)	8	31
All	All	1354/1390 (97%)	1236 (91%)	118 (9%)	13	43

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	81	GLN
1	A	90	ASN
1	A	97	LEU
1	A	98	GLN
1	A	122	THR
1	A	125	THR
1	A	139	GLN
1	A	143	LEU
1	A	149	ASN
1	A	212	VAL
1	A	240	LEU
1	A	259	ILE
1	A	271	TRP
1	A	281	LEU
1	A	287	GLN
1	A	334	THR
1	A	375	GLU

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Mol	Chain	Res	Type
1	A	381	TYR
1	A	385	TYR
1	A	401	HIS
1	A	407	ILE
1	A	418	LEU
1	A	431	ASP
1	A	436	ILE
1	A	438	PHE
1	A	439	LEU
1	A	440	LEU
1	A	441	LYS
1	A	444	LEU
1	A	455	MET
1	A	456	LEU
1	A	473	TRP
1	A	506	VAL
1	A	520	LEU
1	A	524	GLN
1	A	526	GLN
1	A	546	ASN
1	A	549	GLU
1	A	557	MET
1	A	558	LEU
1	A	570	LEU
1	A	573	VAL
1	A	603	PHE
1	B	61	ASN
1	B	81	GLN
1	B	90	ASN
1	B	97	LEU
1	B	98	GLN
1	B	111	ASP
1	B	122	THR
1	B	139	GLN
1	B	212	VAL
1	B	240	LEU
1	B	259	ILE
1	B	271	TRP
1	B	281	LEU
1	B	287	GLN
1	B	290	ASN
1	B	298	VAL

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Mol	Chain	Res	Type
1	B	334	THR
1	B	375	GLU
1	B	381	TYR
1	B	385	TYR
1	B	401	HIS
1	B	407	ILE
1	B	418	LEU
1	B	441	LYS
1	B	444	LEU
1	B	450	LEU
1	B	455	MET
1	B	473	TRP
1	B	477	TRP
1	B	483	GLU
1	B	493	HIS
1	B	494	ASP
1	B	495	GLU
1	B	526	GLN
1	B	536	GLU
1	B	552	GLN
1	B	553	LYS
1	B	557	MET
1	B	559	ARG
1	B	568	LEU
1	B	580	ASN
1	B	592	PHE
1	B	597	ASP
1	B	609	ASP
2	E	333	LYS
2	E	337	VAL
2	E	341	GLU
2	E	348	CYS
2	E	356	TYR
2	E	360	PHE
2	E	361	PHE
2	E	364	PHE
2	E	369	VAL
2	E	405	ILE
2	E	416	PHE
2	E	417	MET
2	E	423	TRP
2	E	467	CYS

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Mol	Chain	Res	Type
2	F	333	LYS
2	F	337	VAL
2	F	341	GLU
2	F	348	CYS
2	F	356	TYR
2	F	357	ASN
2	F	360	PHE
2	F	364	PHE
2	F	367	TYR
2	F	369	VAL
2	F	405	ILE
2	F	416	PHE
2	F	417	MET
2	F	423	TRP
2	F	467	CYS
2	F	481	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	60	GLN
1	A	64	ASN
1	A	81	GLN
1	A	86	GLN
1	A	90	ASN
1	A	96	GLN
1	A	101	GLN
1	A	103	ASN
1	A	139	GLN
1	A	149	ASN
1	A	221	GLN
1	A	290	ASN
1	A	300	GLN
1	A	325	GLN
1	A	330	ASN
1	A	493	HIS
1	A	505	HIS
1	A	508	ASN
1	A	531	GLN
1	A	535	HIS
1	A	540	HIS

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Mol	Chain	Res	Type
1	A	546	ASN
1	A	572	ASN
1	A	586	ASN
1	A	599	ASN
1	B	33	ASN
1	B	49	ASN
1	B	60	GLN
1	B	64	ASN
1	B	81	GLN
1	B	89	GLN
1	B	90	ASN
1	B	98	GLN
1	B	101	GLN
1	B	103	ASN
1	B	139	GLN
1	B	149	ASN
1	B	188	ASN
1	B	210	ASN
1	B	221	GLN
1	B	277	ASN
1	B	290	ASN
1	B	300	GLN
1	B	325	GLN
1	B	373	HIS
1	B	397	ASN
1	B	442	GLN
1	B	472	GLN
1	B	493	HIS
1	B	524	GLN
1	B	526	GLN
1	B	535	HIS
1	B	552	GLN
1	B	572	ASN
1	B	586	ASN
1	B	599	ASN
1	B	601	ASN
2	E	347	ASN
2	E	375	ASN
2	E	409	ASN
2	F	330	ASN
2	F	375	ASN
2	F	409	ASN

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Mol	Chain	Res	Type
2	F	445	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 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	597/603 (99%)	-0.11	3 (0%) 91 76	56, 98, 143, 159	0
1	B	597/603 (99%)	0.00	9 (1%) 76 49	55, 99, 144, 158	0
2	E	173/185 (93%)	0.22	12 (6%) 20 7	79, 116, 149, 157	0
2	F	173/185 (93%)	0.19	7 (4%) 42 17	81, 117, 148, 157	0
All	All	1540/1576 (97%)	0.00	31 (2%) 68 39	55, 103, 146, 159	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	615	ASP	10.4
1	B	105	SER	5.0
2	E	501	PHE	4.2
2	E	421	LEU	4.2
1	A	105	SER	3.4
2	F	475	TYR	3.2
2	F	354	VAL	3.1
2	E	499	LEU	3.1
1	B	89	GLN	3.0
2	E	355	LEU	2.9
2	E	345	ILE	2.6
1	B	614	ALA	2.6
2	F	443	LEU	2.5
2	E	383	TYR	2.5
1	B	97	LEU	2.5
2	E	325	PHE	2.5
1	B	142	LEU	2.4
2	E	412	LEU	2.4
1	B	132	VAL	2.3
2	F	421	LEU	2.3
2	E	357	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
2	F	423	TRP	2.2
2	F	445	HIS	2.2
1	A	615	ASP	2.2
2	E	382	VAL	2.2
1	B	511	SER	2.1
2	E	367	TYR	2.1
2	E	420	VAL	2.0
1	A	86	GLN	2.0
2	F	364	PHE	2.0
1	B	59	VAL	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( $\text{\AA}^2$ )	Q<0.9
4	CL	A	902	1/1	0.89	0.61	9.95	138,138,138,138	0
4	CL	B	902	1/1	0.95	0.28	1.81	108,108,108,108	0
3	ZN	B	901	1/1	0.96	0.46	-	98,98,98,98	0
3	ZN	A	901	1/1	0.96	0.46	-	102,102,102,102	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.