



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:12 AM UTC

PDB ID : 5FMO / pdb_00005fmo
Title : Crystal structure and proteomics analysis of empty virus like particles of Cowpea mosaic virus
Authors : Huynh, N.; Hesketh, E.L.; Saxena, P.; Meshcheriakova, Y.; Ku, Y.C.; Hoang, L.; Johnson, J.E.; Ranson, N.A.; Lomonossoff, G.P.; Reddy, V.S.
Deposited on : 2015-11-07
Resolution : 2.30 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	FAILED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

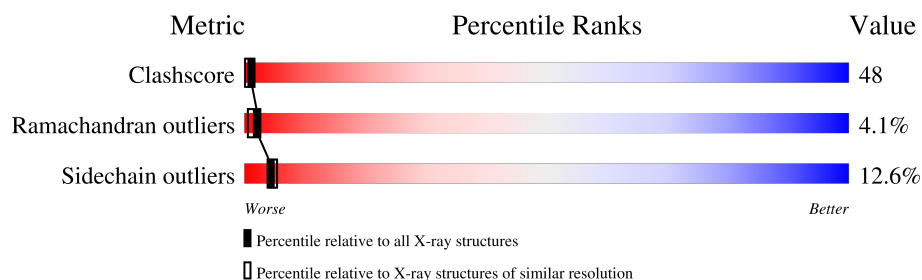
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

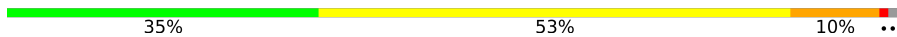
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	L	374	
2	S	213	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4440 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 EMPTY VIRUS LIKE PARTICLES OF COWPEA MOSAIC VIRUS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	370	Total	C	N	O	S	0	0	1
			2866	1822	481	541	22			

- Molecule 2 is a protein called EMPTY VIRUS LIKE PARTICLES OF COWPEA MOSAIC VIRUS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S	194	Total	C	N	O	S	0	0	1
			1516	971	256	280	9			

- Molecule 3 is water.

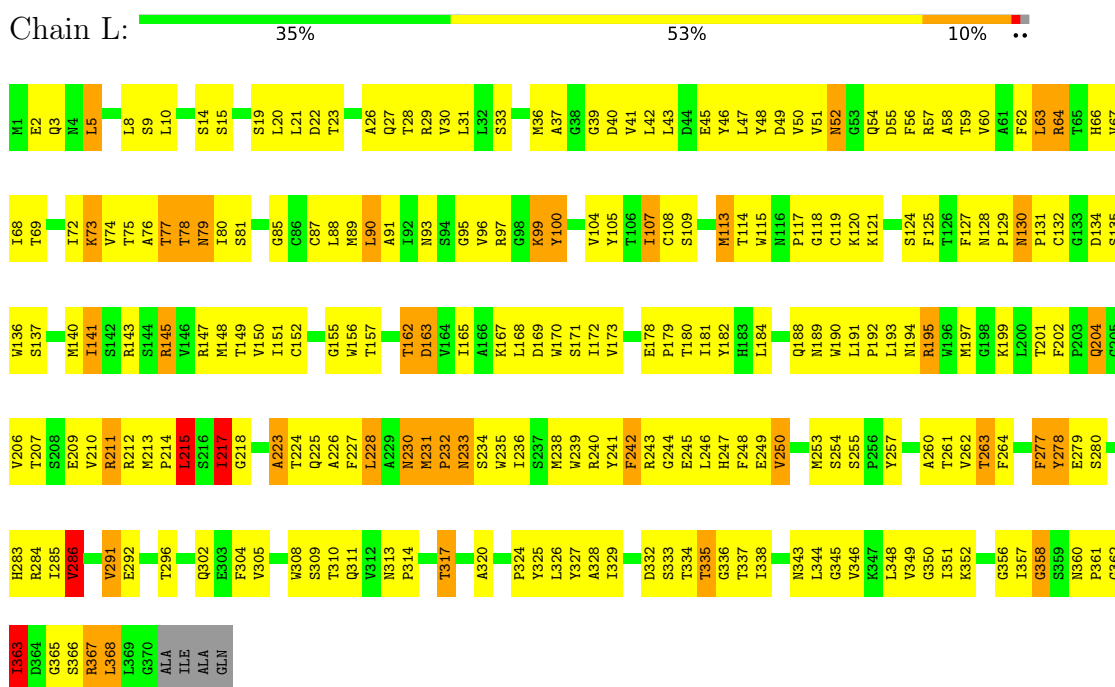
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	45	Total	O	0	0
			45	45		
3	S	13	Total	O	0	0
			13	13		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS failed to run properly.

- Molecule 1: EMPTY VIRUS LIKE PARTICLES OF COWPEA MOSAIC VIRUS



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	655.97Å 655.97Å 571.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.30	Depositor
% Data completeness (in resolution range)	58.3 (10.00-2.30)	Depositor
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.29Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.359 , 0.362	Depositor
Wilson B-factor (Å ²)	7.7	Xtriage
Anisotropy	0.283	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.32$, $\langle L^2 \rangle = 0.15$	Xtriage
Estimated twinning fraction	0.105 for -k,-h,-l	Xtriage
Total number of atoms	4440	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	L	0.56	0/2933	1.04	18/3985 (0.5%)
2	S	0.65	1/1564 (0.1%)	1.19	16/2143 (0.7%)
All	All	0.59	1/4497 (0.0%)	1.10	34/6128 (0.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	562	PRO	N-CA	-6.54	1.39	1.47

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	384	VAL	CB-CA-C	-15.39	91.82	110.91
2	S	561	PRO	CB-CA-C	-9.72	99.06	110.92
1	L	361	PRO	CB-CA-C	-8.82	99.24	112.11
2	S	383	ASP	CA-C-N	7.91	132.57	122.37
2	S	383	ASP	C-N-CA	7.91	132.57	122.37
2	S	387	PRO	CB-CA-C	-7.53	101.75	111.46
2	S	503	SER	N-CA-C	-7.50	101.66	111.71
1	L	368	LEU	N-CA-C	7.37	121.00	107.73
1	L	209	GLU	N-CA-C	7.37	120.93	109.07
1	L	286	VAL	N-CA-C	6.98	117.94	107.75
1	L	291	VAL	N-CA-C	6.91	117.50	111.90
2	S	532	GLN	N-CA-C	6.73	118.78	108.42
2	S	500	GLY	CA-C-N	6.60	126.22	119.56
2	S	500	GLY	C-N-CA	6.60	126.22	119.56
2	S	561	PRO	N-CA-C	6.47	118.59	110.70
1	L	157	THR	N-CA-C	-6.19	104.99	112.54
2	S	382	SER	CA-C-N	5.80	132.63	121.54
2	S	382	SER	C-N-CA	5.80	132.63	121.54
1	L	163	ASP	N-CA-C	-5.79	102.88	110.53
2	S	473	ASN	CA-C-N	5.76	127.05	119.84
2	S	473	ASN	C-N-CA	5.76	127.05	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	215	LEU	N-CA-C	-5.76	106.02	113.16
2	S	509	GLU	N-CA-C	5.67	119.49	112.24
1	L	107	ILE	N-CA-C	5.66	120.33	112.35
1	L	130	ASN	CA-C-N	5.57	125.28	119.82
1	L	130	ASN	C-N-CA	5.57	125.28	119.82
1	L	134	ASP	N-CA-C	-5.53	105.53	114.09
1	L	64	ARG	N-CA-C	5.44	119.63	113.15
2	S	514	ASN	N-CA-C	-5.35	104.04	111.52
1	L	278	TYR	N-CA-C	-5.32	105.48	111.28
1	L	115	TRP	N-CA-C	5.27	116.15	108.14
1	L	178	GLU	CA-C-N	5.22	125.19	120.03
1	L	178	GLU	C-N-CA	5.22	125.19	120.03
1	L	121	LYS	N-CA-C	5.08	121.61	110.80

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	L	2866	0	2813	287	0
2	S	1516	0	1456	147	0
3	L	45	0	0	22	0
3	S	13	0	0	7	0
All	All	4440	0	4269	417	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 48.

All (417) 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:L:22:ASP:O	1:L:58:ALA:HB2	1.60	1.01
1:L:113:MET:HE3	1:L:125:PHE:HD1	1.27	0.96
1:L:113:MET:HE3	1:L:125:PHE:CD1	2.02	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:466:VAL:CG2	2:S:482:PHE:HB2	2.03	0.89
1:L:96:VAL:HG12	2:S:550:LEU:HB2	1.55	0.87
1:L:37:ALA:O	1:L:155:GLY:N	2.07	0.87
2:S:447:GLN:HG3	2:S:493:ASN:HD21	1.40	0.86
1:L:263:THR:HB	1:L:285:ILE:HD13	1.57	0.86
1:L:30:VAL:HG22	1:L:43:LEU:HD13	1.55	0.86
3:L:2018:HOH:O	2:S:502:ASN:HB3	1.75	0.86
2:S:566:PHE:O	2:S:567:ARG:HB2	1.77	0.85
1:L:120:LYS:NZ	3:L:2016:HOH:O	2.11	0.84
1:L:313:ASN:HD22	1:L:314:PRO:N	1.76	0.83
2:S:398:PHE:HE1	2:S:400:ASP:HB2	1.43	0.82
1:L:313:ASN:HA	1:L:363:ILE:HD11	1.62	0.82
2:S:466:VAL:HG23	2:S:482:PHE:HB2	1.61	0.81
2:S:484:ILE:HD12	2:S:484:ILE:O	1.81	0.81
1:L:36:MET:O	1:L:155:GLY:HA2	1.80	0.81
1:L:97:ARG:HB3	2:S:551:MET:HE1	1.62	0.81
1:L:36:MET:HB2	1:L:40:ASP:OD2	1.81	0.80
2:S:450:VAL:HG23	2:S:490:ALA:H	1.47	0.79
1:L:343:ASN:HB2	3:L:2034:HOH:O	1.82	0.78
1:L:199:LYS:HE2	1:L:343:ASN:ND2	1.98	0.78
1:L:2:GLU:HG2	1:L:3:GLN:N	1.97	0.78
2:S:389:MET:HE2	2:S:406:PHE:HD1	1.49	0.77
1:L:199:LYS:HE2	1:L:343:ASN:HD22	1.49	0.77
2:S:428:PRO:HD2	2:S:431:MET:HB2	1.67	0.77
1:L:26:ALA:HB3	1:L:170:TRP:HB2	1.65	0.76
2:S:528:ARG:HA	2:S:528:ARG:NH1	2.00	0.76
2:S:463:GLN:HB2	2:S:525:THR:OG1	1.86	0.75
1:L:59:THR:O	1:L:62:PHE:HB3	1.87	0.75
2:S:447:GLN:HG3	2:S:493:ASN:ND2	2.02	0.74
1:L:305:VAL:HG23	3:L:2043:HOH:O	1.88	0.74
2:S:408:LEU:HB3	2:S:537:MET:HE1	1.70	0.73
1:L:218:GLY:HA3	1:L:311:GLN:HB3	1.71	0.72
1:L:210:VAL:C	1:L:211:ARG:HD2	2.14	0.72
1:L:253:MET:HG3	3:L:2033:HOH:O	1.88	0.72
2:S:465:PHE:HB2	2:S:523:VAL:CG1	2.20	0.72
1:L:228:LEU:HD12	1:L:228:LEU:H	1.53	0.72
1:L:75:THR:HA	1:L:124:SER:HB3	1.71	0.72
1:L:140:MET:HA	2:S:512:TRP:CZ3	2.24	0.71
1:L:141:ILE:HD13	1:L:141:ILE:H	1.55	0.71
1:L:230:ASN:HD21	1:L:233:ASN:HB3	1.55	0.71
2:S:471:SER:HA	2:S:519:TYR:CE2	2.26	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:560:THR:C	2:S:562:PRO:HD2	2.16	0.71
1:L:23:THR:HG22	1:L:171:SER:HB3	1.71	0.70
2:S:471:SER:HA	2:S:519:TYR:HE2	1.56	0.70
1:L:215:LEU:HD23	1:L:325:TYR:HA	1.75	0.69
1:L:277:PHE:HD1	1:L:277:PHE:N	1.89	0.69
1:L:231:MET:HE2	1:L:232:PRO:N	2.07	0.69
1:L:217:ILE:H	1:L:217:ILE:HD13	1.58	0.69
1:L:277:PHE:N	1:L:277:PHE:CD1	2.59	0.68
1:L:313:ASN:HD22	1:L:313:ASN:C	2.02	0.68
1:L:223:ALA:HB3	1:L:226:ALA:O	1.94	0.68
1:L:235:TRP:O	1:L:238:MET:HG2	1.94	0.68
1:L:261:THR:HB	1:L:332:ASP:OD1	1.94	0.68
2:S:385:TYR:C	3:S:2003:HOH:O	2.36	0.68
1:L:93:ASN:HD22	2:S:548:ASN:HD22	1.41	0.68
2:S:450:VAL:O	2:S:489:SER:HB2	1.94	0.68
1:L:230:ASN:C	1:L:230:ASN:HD22	2.01	0.67
2:S:403:ALA:HB2	2:S:523:VAL:HG23	1.76	0.67
1:L:33:SER:H	1:L:36:MET:HE1	1.60	0.67
2:S:524:ALA:HB1	2:S:530:ILE:HD12	1.77	0.66
1:L:93:ASN:ND2	2:S:548:ASN:HD22	1.92	0.66
2:S:428:PRO:HD2	2:S:431:MET:CB	2.25	0.66
1:L:33:SER:H	1:L:36:MET:CE	2.08	0.66
1:L:130:ASN:C	1:L:130:ASN:HD22	2.02	0.65
1:L:47:LEU:O	1:L:50:VAL:HG12	1.97	0.65
1:L:231:MET:HB3	1:L:232:PRO:HD3	1.79	0.65
1:L:230:ASN:HD21	1:L:233:ASN:CB	2.09	0.65
2:S:481:THR:HA	3:S:2007:HOH:O	1.97	0.65
1:L:37:ALA:HA	1:L:155:GLY:HA3	1.79	0.64
2:S:486:GLN:HG3	2:S:490:ALA:HB2	1.78	0.64
1:L:48:TYR:O	1:L:51:VAL:HG22	1.98	0.64
1:L:42:LEU:HD21	1:L:152:CYS:HB2	1.79	0.64
1:L:99:LYS:O	2:S:552:PRO:HB3	1.97	0.64
1:L:231:MET:HE2	1:L:232:PRO:CA	2.28	0.64
1:L:45:GLU:C	1:L:147:ARG:HH11	2.06	0.64
1:L:230:ASN:ND2	1:L:233:ASN:HB3	2.11	0.64
2:S:500:GLY:HA3	2:S:505:PHE:C	2.22	0.64
2:S:388:CYS:HB3	2:S:431:MET:SD	2.37	0.64
1:L:162:THR:HG22	1:L:163:ASP:H	1.63	0.63
1:L:206:VAL:HG12	1:L:206:VAL:O	1.98	0.63
1:L:225:GLN:HA	1:L:225:GLN:NE2	2.14	0.63
1:L:46:TYR:N	1:L:147:ARG:HH11	1.95	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:225:GLN:HA	1:L:225:GLN:HE21	1.63	0.63
1:L:214:PRO:HA	1:L:325:TYR:CE1	2.34	0.63
2:S:443:THR:HG23	2:S:542:ASN:HD21	1.64	0.63
1:L:231:MET:HE2	1:L:232:PRO:HA	1.81	0.63
1:L:260:ALA:HB2	1:L:334:THR:HA	1.81	0.63
2:S:465:PHE:HB2	2:S:523:VAL:HG12	1.81	0.63
1:L:36:MET:O	1:L:36:MET:HG3	1.99	0.62
2:S:563:LEU:O	2:S:565:LYS:HG2	1.99	0.62
1:L:45:GLU:HA	1:L:147:ARG:NH1	2.14	0.62
1:L:97:ARG:CB	2:S:551:MET:HE1	2.29	0.62
1:L:33:SER:HB3	1:L:36:MET:HE2	1.80	0.62
1:L:74:VAL:HA	3:L:2007:HOH:O	1.98	0.62
1:L:231:MET:HE2	1:L:231:MET:C	2.23	0.62
1:L:15:SER:OG	1:L:69:THR:HG22	1.99	0.62
1:L:193:LEU:HD11	1:L:351:ILE:HG12	1.81	0.62
1:L:313:ASN:HD22	1:L:314:PRO:CD	2.13	0.62
2:S:448:LEU:HB3	2:S:492:LEU:CD1	2.30	0.62
2:S:430:ILE:O	2:S:433:VAL:HG22	1.99	0.61
1:L:113:MET:HE2	1:L:124:SER:HA	1.82	0.61
2:S:561:PRO:O	2:S:562:PRO:C	2.39	0.61
1:L:217:ILE:HD13	1:L:217:ILE:N	2.16	0.61
2:S:563:LEU:O	2:S:565:LYS:N	2.34	0.61
2:S:405:THR:HG21	2:S:472:MET:HE2	1.82	0.60
1:L:72:ILE:HD11	1:L:136:TRP:CZ2	2.36	0.60
1:L:23:THR:CG2	1:L:172:ILE:H	2.14	0.60
2:S:450:VAL:HG12	2:S:533:PHE:CD1	2.36	0.60
1:L:141:ILE:HD13	1:L:141:ILE:N	2.16	0.60
1:L:329:ILE:HD12	1:L:329:ILE:N	2.15	0.60
2:S:528:ARG:HA	2:S:528:ARG:CZ	2.31	0.60
1:L:5:LEU:HD12	1:L:5:LEU:H	1.66	0.60
1:L:313:ASN:ND2	1:L:314:PRO:HD2	2.17	0.60
2:S:509:GLU:HG3	2:S:517:THR:HB	1.84	0.59
2:S:560:THR:N	2:S:561:PRO:CD	2.66	0.59
1:L:227:PHE:CD2	1:L:365:GLY:HA2	2.38	0.59
1:L:80:ILE:HG23	1:L:118:GLY:HA2	1.85	0.59
1:L:217:ILE:H	1:L:217:ILE:CD1	2.15	0.59
1:L:46:TYR:HB2	1:L:49:ASP:OD2	2.03	0.59
1:L:195:ARG:HD3	1:L:233:ASN:OD1	2.03	0.59
1:L:80:ILE:HD12	1:L:81:SER:H	1.67	0.59
1:L:135:SER:HA	3:L:2006:HOH:O	2.01	0.59
2:S:492:LEU:HD13	2:S:492:LEU:O	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:245:GLU:HB3	1:L:352:LYS:HB3	1.84	0.58
1:L:190:TRP:HE1	1:L:192:PRO:HG3	1.67	0.58
2:S:466:VAL:C	2:S:467:TYR:HD1	2.11	0.58
2:S:559:GLU:HB3	2:S:561:PRO:HD2	1.86	0.58
1:L:233:ASN:C	1:L:233:ASN:HD22	2.12	0.58
2:S:451:ARG:HD2	2:S:532:GLN:OE1	2.04	0.58
1:L:344:LEU:HA	3:L:2033:HOH:O	2.04	0.58
1:L:304:PHE:HB2	3:L:2030:HOH:O	2.04	0.57
1:L:63:LEU:HD22	1:L:63:LEU:H	1.69	0.57
1:L:113:MET:CE	1:L:125:PHE:HD1	2.10	0.57
1:L:28:THR:HG21	1:L:50:VAL:HG23	1.85	0.57
2:S:517:THR:HG23	2:S:518:TRP:N	2.18	0.57
1:L:332:ASP:CG	1:L:333:SER:H	2.12	0.57
2:S:566:PHE:O	2:S:567:ARG:CB	2.51	0.57
1:L:181:ILE:N	1:L:181:ILE:HD12	2.19	0.56
2:S:464:VAL:HB	2:S:484:ILE:HD11	1.87	0.56
1:L:137:SER:O	1:L:140:MET:HB3	2.05	0.56
1:L:253:MET:N	3:L:2033:HOH:O	2.36	0.56
1:L:190:TRP:NE1	1:L:192:PRO:HG3	2.21	0.56
1:L:233:ASN:O	1:L:236:ILE:HG22	2.06	0.56
1:L:21:LEU:O	1:L:21:LEU:HD23	2.05	0.56
1:L:88:LEU:CD2	1:L:117:PRO:HD3	2.36	0.56
2:S:551:MET:HE2	2:S:551:MET:HA	1.88	0.56
1:L:23:THR:CG2	1:L:172:ILE:N	2.69	0.56
1:L:104:VAL:HG13	1:L:105:TYR:N	2.20	0.56
2:S:460:TRP:HA	2:S:529:GLN:HE22	1.69	0.56
1:L:193:LEU:HD12	1:L:350:GLY:HA2	1.88	0.56
1:L:213:MET:O	1:L:325:TYR:HD1	1.88	0.55
1:L:149:THR:HG22	1:L:150:VAL:N	2.21	0.55
1:L:253:MET:HE2	1:L:345:GLY:N	2.22	0.55
1:L:357:ILE:N	1:L:357:ILE:HD12	2.22	0.55
2:S:452:GLY:HA2	2:S:531:GLN:H	1.71	0.55
1:L:43:LEU:HD23	1:L:43:LEU:C	2.31	0.55
1:L:76:ALA:HA	1:L:167:LYS:O	2.07	0.55
1:L:263:THR:HB	1:L:285:ILE:CD1	2.31	0.55
1:L:87:CYS:HB2	1:L:253:MET:HB3	1.87	0.55
1:L:113:MET:CE	1:L:124:SER:HA	2.36	0.55
2:S:389:MET:HG2	2:S:425:ILE:HD12	1.89	0.55
2:S:455:VAL:HG11	2:S:529:GLN:HE21	1.71	0.55
1:L:225:GLN:HA	2:S:556:LEU:HD12	1.89	0.54
2:S:443:THR:HG22	2:S:497:ASP:CG	2.31	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:90:LEU:HD22	1:L:150:VAL:HG22	1.89	0.54
1:L:109:SER:HB3	1:L:230:ASN:OD1	2.07	0.54
1:L:42:LEU:HB2	1:L:150:VAL:HG12	1.87	0.54
1:L:128:ASN:C	1:L:128:ASN:HD22	2.16	0.54
2:S:448:LEU:HD23	2:S:449:ASN:N	2.23	0.54
2:S:398:PHE:CE1	2:S:400:ASP:HB2	2.34	0.54
2:S:465:PHE:O	2:S:523:VAL:HG12	2.08	0.54
1:L:349:VAL:N	3:L:2031:HOH:O	2.38	0.54
2:S:431:MET:O	2:S:435:ARG:HD3	2.07	0.54
2:S:394:PRO:HA	2:S:420:ASN:O	2.07	0.53
2:S:389:MET:HB3	2:S:413:ILE:HD11	1.90	0.53
1:L:365:GLY:O	1:L:366:SER:HB3	2.09	0.53
1:L:63:LEU:HD22	1:L:63:LEU:N	2.24	0.53
2:S:528:ARG:NH1	3:S:2004:HOH:O	2.41	0.53
1:L:167:LYS:C	1:L:168:LEU:HD22	2.33	0.53
1:L:145:ARG:HB2	1:L:145:ARG:HH11	1.73	0.53
1:L:143:ARG:C	1:L:145:ARG:H	2.15	0.52
2:S:506:GLU:C	3:S:2006:HOH:O	2.52	0.52
1:L:108:CYS:O	1:L:194:ASN:HB3	2.09	0.52
1:L:169:ASP:C	3:L:2007:HOH:O	2.52	0.52
2:S:430:ILE:HG13	2:S:539:PHE:CE2	2.44	0.52
1:L:149:THR:HG22	1:L:150:VAL:H	1.75	0.52
1:L:45:GLU:CA	1:L:147:ARG:HH11	2.23	0.52
1:L:313:ASN:HA	1:L:363:ILE:CD1	2.38	0.52
2:S:561:PRO:N	2:S:562:PRO:CD	2.72	0.52
1:L:233:ASN:C	1:L:233:ASN:ND2	2.68	0.52
2:S:460:TRP:HA	2:S:529:GLN:NE2	2.25	0.52
1:L:28:THR:CG2	1:L:50:VAL:HG23	2.39	0.52
1:L:239:TRP:C	1:L:360:ASN:HB2	2.34	0.52
1:L:249:GLU:N	3:L:2032:HOH:O	2.42	0.52
1:L:89:MET:CE	1:L:91:ALA:HB2	2.40	0.52
1:L:72:ILE:HD13	1:L:129:PRO:HD3	1.92	0.51
1:L:95:GLY:O	2:S:549:ILE:HA	2.10	0.51
2:S:389:MET:HE2	2:S:406:PHE:CD1	2.38	0.51
1:L:349:VAL:HB	3:L:2031:HOH:O	2.11	0.51
1:L:33:SER:N	1:L:36:MET:CE	2.73	0.51
1:L:73:LYS:HD3	1:L:75:THR:OG1	2.10	0.51
1:L:362:GLY:HA3	2:S:429:PRO:HD3	1.93	0.51
1:L:90:LEU:HD21	1:L:148:MET:HE1	1.92	0.51
1:L:45:GLU:HA	1:L:147:ARG:HH11	1.76	0.51
1:L:68:ILE:HD13	1:L:137:SER:HA	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:239:TRP:O	1:L:310:THR:HG21	2.10	0.51
1:L:193:LEU:HD21	1:L:236:ILE:HD12	1.93	0.50
1:L:211:ARG:HD2	1:L:211:ARG:N	2.25	0.50
1:L:85:GLY:N	1:L:255:SER:HB2	2.26	0.50
2:S:438:ALA:HB2	2:S:549:ILE:HG23	1.93	0.50
1:L:2:GLU:HG2	1:L:3:GLN:H	1.75	0.50
1:L:113:MET:HE2	1:L:124:SER:CA	2.40	0.50
1:L:197:MET:HB2	1:L:346:VAL:O	2.11	0.50
1:L:72:ILE:HD12	1:L:72:ILE:N	2.27	0.50
1:L:254:SER:N	3:L:2034:HOH:O	2.44	0.50
1:L:313:ASN:ND2	1:L:314:PRO:CD	2.75	0.50
1:L:23:THR:HG22	1:L:172:ILE:H	1.77	0.50
1:L:248:PHE:CE1	1:L:348:LEU:HB2	2.47	0.50
2:S:396:ALA:HA	3:S:2004:HOH:O	2.12	0.50
1:L:214:PRO:HA	1:L:325:TYR:CD1	2.47	0.49
1:L:311:GLN:CD	1:L:363:ILE:CG2	2.85	0.49
1:L:36:MET:O	1:L:36:MET:CG	2.61	0.49
1:L:8:LEU:C	1:L:10:LEU:H	2.18	0.49
1:L:141:ILE:H	1:L:141:ILE:CD1	2.22	0.49
2:S:389:MET:HG2	2:S:425:ILE:CD1	2.42	0.49
1:L:231:MET:HB2	2:S:436:THR:O	2.13	0.49
1:L:64:ARG:HD2	1:L:64:ARG:N	2.28	0.48
1:L:68:ILE:HG21	1:L:136:TRP:CZ2	2.48	0.48
1:L:88:LEU:HD22	1:L:88:LEU:N	2.28	0.48
2:S:448:LEU:HB3	2:S:492:LEU:HD13	1.95	0.48
1:L:128:ASN:HD22	1:L:129:PRO:HD2	1.77	0.48
1:L:212:ARG:HG3	1:L:212:ARG:HH11	1.78	0.48
2:S:450:VAL:HG12	2:S:533:PHE:HD1	1.76	0.48
2:S:559:GLU:C	2:S:561:PRO:HD2	2.39	0.48
1:L:356:GLY:C	1:L:357:ILE:HD12	2.37	0.48
2:S:544:ARG:HG3	2:S:544:ARG:HH11	1.79	0.48
1:L:328:ALA:C	1:L:329:ILE:HD12	2.39	0.48
2:S:484:ILE:HD12	2:S:484:ILE:C	2.37	0.48
2:S:435:ARG:HD3	2:S:435:ARG:H	1.79	0.48
1:L:128:ASN:C	1:L:128:ASN:ND2	2.70	0.47
1:L:130:ASN:C	1:L:130:ASN:ND2	2.71	0.47
1:L:255:SER:C	1:L:257:TYR:H	2.21	0.47
1:L:335:THR:OG1	1:L:336:GLY:N	2.47	0.47
2:S:462:GLY:O	2:S:463:GLN:HG3	2.13	0.47
2:S:465:PHE:HB3	2:S:467:TYR:HE1	1.78	0.47
2:S:387:PRO:O	2:S:428:PRO:HG2	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:50:VAL:HG21	1:L:170:TRP:NE1	2.30	0.47
1:L:211:ARG:HH11	1:L:211:ARG:HG2	1.79	0.47
2:S:496:PHE:CD1	2:S:496:PHE:N	2.83	0.47
1:L:42:LEU:HD23	1:L:151:ILE:C	2.40	0.47
1:L:179:PRO:HB2	1:L:181:ILE:CD1	2.45	0.47
1:L:253:MET:HE2	1:L:344:LEU:C	2.39	0.47
2:S:430:ILE:HD13	2:S:537:MET:O	2.14	0.47
1:L:59:THR:O	1:L:63:LEU:CD2	2.63	0.47
1:L:128:ASN:HD22	1:L:129:PRO:CD	2.28	0.47
1:L:184:LEU:HD11	2:S:543:PHE:HB3	1.96	0.47
2:S:403:ALA:O	2:S:416:VAL:HG22	2.15	0.47
1:L:29:ARG:NH1	1:L:29:ARG:HG3	2.31	0.46
1:L:284:ARG:HG3	1:L:284:ARG:HH11	1.80	0.46
2:S:443:THR:HG22	2:S:497:ASP:OD2	2.14	0.46
2:S:500:GLY:HA3	2:S:505:PHE:O	2.14	0.46
1:L:250:VAL:HG13	1:L:346:VAL:HG22	1.97	0.46
1:L:255:SER:C	1:L:257:TYR:N	2.73	0.46
2:S:413:ILE:HG13	2:S:425:ILE:HD11	1.98	0.46
1:L:73:LYS:HB2	1:L:173:VAL:CG1	2.46	0.46
1:L:246:LEU:HD13	1:L:351:ILE:HD12	1.98	0.46
2:S:406:PHE:O	2:S:519:TYR:HA	2.16	0.46
2:S:537:MET:N	3:S:2003:HOH:O	2.47	0.46
1:L:262:VAL:O	1:L:286:VAL:HG23	2.15	0.46
1:L:75:THR:HG23	1:L:124:SER:HB3	1.96	0.46
1:L:88:LEU:HD23	1:L:117:PRO:HD3	1.98	0.46
1:L:89:MET:HE1	1:L:108:CYS:HB3	1.98	0.46
1:L:193:LEU:HD12	1:L:193:LEU:N	2.30	0.46
2:S:561:PRO:C	2:S:562:PRO:O	2.55	0.46
1:L:162:THR:HG22	1:L:163:ASP:N	2.30	0.46
2:S:398:PHE:C	2:S:398:PHE:CD1	2.92	0.46
1:L:367:ARG:H	1:L:367:ARG:HG2	1.51	0.46
1:L:19:SER:C	1:L:21:LEU:H	2.24	0.46
2:S:551:MET:HB3	2:S:552:PRO:HD2	1.98	0.46
2:S:493:ASN:N	2:S:493:ASN:HD22	2.14	0.45
2:S:450:VAL:HG12	2:S:533:PHE:CE1	2.51	0.45
1:L:73:LYS:HB2	1:L:173:VAL:HG13	1.98	0.45
1:L:226:ALA:HB1	2:S:554:PHE:O	2.16	0.45
1:L:247:HIS:O	1:L:348:LEU:HD12	2.16	0.45
2:S:561:PRO:N	2:S:562:PRO:HD2	2.31	0.45
3:L:2018:HOH:O	2:S:505:PHE:HB2	2.17	0.45
1:L:337:THR:O	1:L:338:ILE:HD13	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:390:ILE:HG22	2:S:424:HIS:HB2	1.98	0.45
1:L:42:LEU:HD22	1:L:42:LEU:H	1.82	0.45
1:L:132:CYS:HA	1:L:181:ILE:HD11	1.99	0.45
2:S:448:LEU:CD1	2:S:466:VAL:HG11	2.47	0.45
1:L:23:THR:HG23	1:L:172:ILE:H	1.82	0.45
1:L:33:SER:N	1:L:36:MET:HE1	2.30	0.45
1:L:311:GLN:OE1	1:L:363:ILE:HG22	2.17	0.45
1:L:362:GLY:CA	2:S:429:PRO:HD3	2.47	0.45
2:S:471:SER:OG	2:S:473:ASN:ND2	2.50	0.45
1:L:317:THR:HG23	1:L:320:ALA:HB3	1.98	0.44
1:L:367:ARG:HE	1:L:367:ARG:HB3	1.64	0.44
2:S:463:GLN:HB2	2:S:525:THR:HG1	1.81	0.44
1:L:23:THR:HG22	1:L:172:ILE:N	2.32	0.44
1:L:148:MET:HE3	1:L:170:TRP:CZ2	2.52	0.44
1:L:223:ALA:N	1:L:368:LEU:HD13	2.32	0.44
1:L:241:TYR:HD1	1:L:309:SER:HA	1.83	0.44
1:L:260:ALA:CB	1:L:334:THR:HA	2.46	0.44
1:L:89:MET:HE3	1:L:91:ALA:HB2	1.99	0.44
1:L:180:THR:C	1:L:181:ILE:HD12	2.43	0.44
2:S:449:ASN:HB2	2:S:534:GLU:HB3	2.00	0.44
1:L:56:PHE:O	1:L:57:ARG:C	2.61	0.44
1:L:143:ARG:C	1:L:145:ARG:N	2.76	0.44
1:L:231:MET:HG3	2:S:437:ALA:HA	2.00	0.43
1:L:327:TYR:HB3	1:L:329:ILE:CD1	2.48	0.43
2:S:389:MET:HE3	2:S:413:ILE:HG13	1.99	0.43
2:S:475:GLU:O	2:S:476:SER:C	2.61	0.43
2:S:427:ASN:N	2:S:428:PRO:HD3	2.32	0.43
1:L:29:ARG:HG3	1:L:29:ARG:HH11	1.83	0.43
1:L:137:SER:O	1:L:141:ILE:CD1	2.66	0.43
1:L:36:MET:O	1:L:155:GLY:CA	2.59	0.43
1:L:96:VAL:HB	1:L:100:TYR:CD2	2.54	0.43
1:L:225:GLN:HE21	1:L:225:GLN:CA	2.25	0.43
2:S:450:VAL:O	2:S:489:SER:CB	2.65	0.43
2:S:457:ARG:O	2:S:459:ASP:N	2.51	0.43
1:L:90:LEU:HD21	1:L:148:MET:CE	2.47	0.43
1:L:244:GLY:O	1:L:246:LEU:HD22	2.19	0.43
2:S:465:PHE:CE1	2:S:483:VAL:HG23	2.54	0.43
1:L:66:HIS:O	1:L:137:SER:HB3	2.18	0.43
1:L:327:TYR:HB3	1:L:329:ILE:HD11	2.01	0.43
2:S:413:ILE:HG21	2:S:423:THR:HG22	2.00	0.43
2:S:562:PRO:O	2:S:563:LEU:C	2.59	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:254:SER:HB3	3:L:2034:HOH:O	2.18	0.43
2:S:426:TYR:C	2:S:428:PRO:HD3	2.44	0.43
2:S:464:VAL:HB	2:S:484:ILE:CD1	2.49	0.43
1:L:77:THR:O	1:L:78:THR:HB	2.18	0.43
1:L:182:TYR:CD2	1:L:231:MET:HE1	2.54	0.43
1:L:197:MET:HE2	1:L:213:MET:HB3	2.01	0.43
2:S:457:ARG:C	2:S:459:ASP:H	2.25	0.43
2:S:460:TRP:CD2	2:S:487:PRO:HA	2.53	0.43
2:S:466:VAL:HG12	2:S:522:CYS:SG	2.59	0.43
2:S:387:PRO:HA	2:S:536:ASN:OD1	2.19	0.43
1:L:85:GLY:HA3	1:L:255:SER:N	2.34	0.43
1:L:326:LEU:HD23	1:L:327:TYR:N	2.34	0.43
2:S:398:PHE:C	2:S:398:PHE:HD1	2.27	0.43
1:L:2:GLU:CG	1:L:3:GLN:N	2.77	0.42
1:L:129:PRO:O	1:L:131:PRO:HD3	2.19	0.42
1:L:148:MET:SD	1:L:148:MET:C	3.02	0.42
1:L:227:PHE:CD1	1:L:227:PHE:C	2.98	0.42
1:L:248:PHE:HE1	1:L:348:LEU:HB2	1.82	0.42
2:S:465:PHE:HB3	2:S:467:TYR:CE1	2.54	0.42
1:L:55:ASP:OD1	1:L:55:ASP:O	2.38	0.42
1:L:62:PHE:CD2	1:L:63:LEU:HD13	2.54	0.42
2:S:439:TRP:HA	3:S:2006:HOH:O	2.19	0.42
1:L:79:ASN:HD22	1:L:79:ASN:HA	1.62	0.42
1:L:95:GLY:HA3	2:S:549:ILE:HG22	2.02	0.42
1:L:100:TYR:O	1:L:100:TYR:HD1	2.02	0.42
2:S:528:ARG:NH1	2:S:528:ARG:CA	2.78	0.42
1:L:130:ASN:HA	1:L:131:PRO:HD2	1.88	0.42
1:L:225:GLN:O	1:L:226:ALA:HB2	2.19	0.42
1:L:250:VAL:HA	1:L:345:GLY:O	2.19	0.42
1:L:264:PHE:CD1	1:L:264:PHE:N	2.86	0.42
1:L:130:ASN:ND2	1:L:132:CYS:H	2.18	0.42
1:L:291:VAL:O	1:L:292:GLU:C	2.63	0.42
2:S:394:PRO:HG3	2:S:398:PHE:CD2	2.55	0.42
1:L:357:ILE:O	1:L:358:GLY:O	2.38	0.42
2:S:472:MET:HG2	2:S:519:TYR:CE2	2.54	0.42
1:L:63:LEU:H	1:L:63:LEU:CD2	2.31	0.42
1:L:263:THR:CB	1:L:285:ILE:HD13	2.38	0.42
1:L:360:ASN:ND2	1:L:362:GLY:HA2	2.35	0.42
1:L:20:LEU:HD23	1:L:20:LEU:O	2.20	0.41
1:L:168:LEU:HD22	1:L:168:LEU:N	2.35	0.41
1:L:264:PHE:O	1:L:283:HIS:HB2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:27:GLN:HA	1:L:168:LEU:O	2.20	0.41
1:L:127:PHE:CD1	1:L:127:PHE:C	2.98	0.41
1:L:242:PHE:HE1	1:L:308:TRP:NE1	2.18	0.41
1:L:333:SER:HA	3:L:2028:HOH:O	2.20	0.41
2:S:430:ILE:HG23	2:S:431:MET:H	1.84	0.41
2:S:560:THR:N	2:S:561:PRO:HD3	2.35	0.41
1:L:78:THR:HG23	1:L:78:THR:O	2.20	0.41
1:L:201:THR:HA	3:L:2027:HOH:O	2.19	0.41
1:L:243:ARG:NH2	3:L:2030:HOH:O	2.54	0.41
2:S:394:PRO:CA	2:S:420:ASN:O	2.67	0.41
2:S:403:ALA:HB2	2:S:523:VAL:CG2	2.46	0.41
1:L:8:LEU:C	1:L:10:LEU:N	2.78	0.41
1:L:230:ASN:HD21	1:L:233:ASN:H	1.68	0.41
1:L:368:LEU:O	1:L:368:LEU:HG	2.20	0.41
2:S:405:THR:CG2	2:S:472:MET:HE2	2.47	0.41
1:L:43:LEU:HD23	1:L:43:LEU:O	2.20	0.41
1:L:59:THR:O	1:L:63:LEU:HD22	2.20	0.41
1:L:247:HIS:C	3:L:2031:HOH:O	2.62	0.41
1:L:41:VAL:O	1:L:41:VAL:HG13	2.20	0.41
1:L:218:GLY:CA	1:L:311:GLN:HB3	2.43	0.41
1:L:51:VAL:O	1:L:52:ASN:C	2.63	0.41
1:L:95:GLY:CA	2:S:549:ILE:HG22	2.51	0.41
1:L:8:LEU:O	1:L:10:LEU:N	2.45	0.41
1:L:21:LEU:HD23	1:L:21:LEU:C	2.46	0.41
1:L:107:ILE:HD11	1:L:151:ILE:HD13	2.02	0.41
1:L:202:PHE:HB3	1:L:334:THR:HG21	2.03	0.41
1:L:278:TYR:C	1:L:280:SER:H	2.29	0.41
2:S:390:ILE:HD13	2:S:391:ALA:N	2.36	0.41
2:S:398:PHE:HD1	2:S:399:SER:N	2.19	0.41
2:S:492:LEU:C	2:S:493:ASN:HD22	2.29	0.41
1:L:204:GLN:HA	1:L:334:THR:OG1	2.21	0.40
1:L:236:ILE:C	1:L:238:MET:H	2.30	0.40
1:L:80:ILE:CG2	1:L:118:GLY:HA2	2.51	0.40
1:L:85:GLY:O	1:L:156:TRP:HA	2.22	0.40
1:L:365:GLY:O	1:L:366:SER:CB	2.68	0.40
2:S:526:ASN:OD1	2:S:528:ARG:HB3	2.21	0.40
1:L:23:THR:HG23	1:L:172:ILE:O	2.21	0.40
1:L:46:TYR:N	1:L:147:ARG:NH1	2.66	0.40
1:L:253:MET:C	3:L:2034:HOH:O	2.64	0.40
2:S:444:ILE:HB	2:S:496:PHE:CE1	2.56	0.40
2:S:552:PRO:O	2:S:553:PRO:C	2.64	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:400:ASP:O	2:S:527:PRO:HG3	2.21	0.40
2:S:446:VAL:HG12	2:S:447:GLN:N	2.37	0.40
1:L:230:ASN:O	1:L:234:SER:HB2	2.21	0.40
2:S:447:GLN:CG	2:S:493:ASN:HD21	2.21	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	L	368/374 (98%)	301 (82%)	54 (15%)	13 (4%)	3	1
2	S	192/213 (90%)	164 (85%)	18 (9%)	10 (5%)	1	1
All	All	560/587 (95%)	465 (83%)	72 (13%)	23 (4%)	2	1

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	39	GLY
1	L	54	GLN
2	S	458	ALA
2	S	567	ARG
1	L	217	ILE
1	L	279	GLU
1	L	358	GLY
1	L	363	ILE
2	S	564	LEU
1	L	78	THR
1	L	99	LYS
1	L	223	ALA
2	S	474	PRO
2	S	502	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	S	512	TRP
1	L	9	SER
1	L	52	ASN
1	L	232	PRO
1	L	324	PRO
2	S	508	ALA
2	S	416	VAL
2	S	487	PRO
2	S	560	THR

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	L	318/320 (99%)	274 (86%)	44 (14%)	3	4
2	S	167/183 (91%)	150 (90%)	17 (10%)	7	8
All	All	485/503 (96%)	424 (87%)	61 (13%)	4	5

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	5	LEU
1	L	14	SER
1	L	31	LEU
1	L	60	VAL
1	L	63	LEU
1	L	67	VAL
1	L	73	LYS
1	L	77	THR
1	L	79	ASN
1	L	90	LEU
1	L	100	TYR
1	L	113	MET
1	L	114	THR
1	L	119	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	141	ILE
1	L	145	ARG
1	L	162	THR
1	L	165	ILE
1	L	188	GLN
1	L	189	ASN
1	L	191	LEU
1	L	195	ARG
1	L	204	GLN
1	L	207	THR
1	L	211	ARG
1	L	215	LEU
1	L	217	ILE
1	L	224	THR
1	L	228	LEU
1	L	230	ASN
1	L	231	MET
1	L	233	ASN
1	L	240	ARG
1	L	242	PHE
1	L	250	VAL
1	L	263	THR
1	L	277	PHE
1	L	286	VAL
1	L	296	THR
1	L	302	GLN
1	L	317	THR
1	L	335	THR
1	L	363	ILE
1	L	367	ARG
2	S	378	CYS
2	S	384	VAL
2	S	390	ILE
2	S	416	VAL
2	S	420	ASN
2	S	435	ARG
2	S	450	VAL
2	S	460	TRP
2	S	486	GLN
2	S	491	MET
2	S	492	LEU
2	S	497	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	S	518	TRP
2	S	528	ARG
2	S	549	ILE
2	S	558	THR
2	S	560	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	3	GLN
1	L	4	ASN
1	L	27	GLN
1	L	52	ASN
1	L	79	ASN
1	L	93	ASN
1	L	128	ASN
1	L	130	ASN
1	L	188	GLN
1	L	204	GLN
1	L	225	GLN
1	L	230	ASN
1	L	287	GLN
1	L	313	ASN
1	L	343	ASN
2	S	410	ASN
2	S	470	GLN
2	S	473	ASN
2	S	486	GLN
2	S	493	ASN
2	S	502	ASN
2	S	529	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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

EDS failed to run properly - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.