



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:22 AM UTC

PDB ID : 1YA0 / pdb_00001ya0
Title : Crystal structure of the N-terminal domain of human SMG7
Authors : Fukuhara, N.; Ebert, J.; Unterholzner, L.; Lindner, D.; Izaurralde, E.; Conti, E.
Deposited on : 2004-12-17
Resolution : 2.55 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

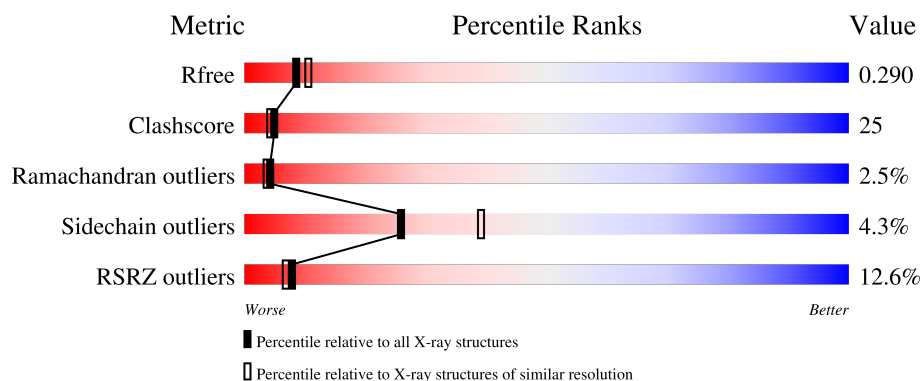
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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 $\leq 5\%$. 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	497	14% 47% 39% 5% • 8%
1	B	497	9% 52% 35% • • 7%

2 Entry composition [i](#)

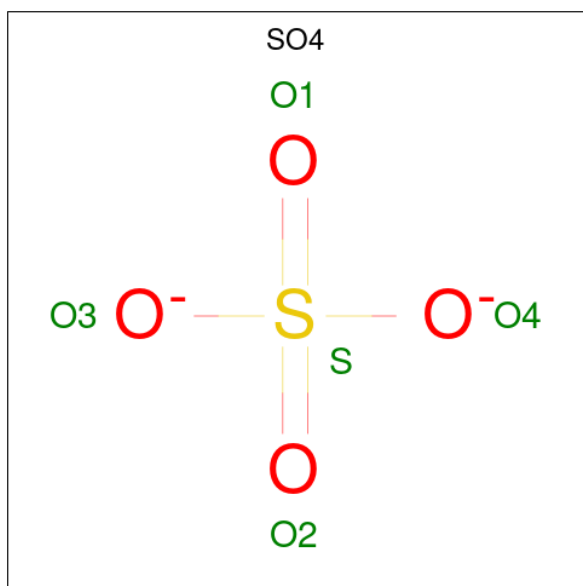
There are 3 unique types of molecules in this entry. The entry contains 7854 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SMG-7 transcript variant 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	458	Total	C	N	O	S	186	0	0
			3737	2384	646	693	14			
1	B	464	Total	C	N	O	S	102	0	0
			3783	2417	650	701	15			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

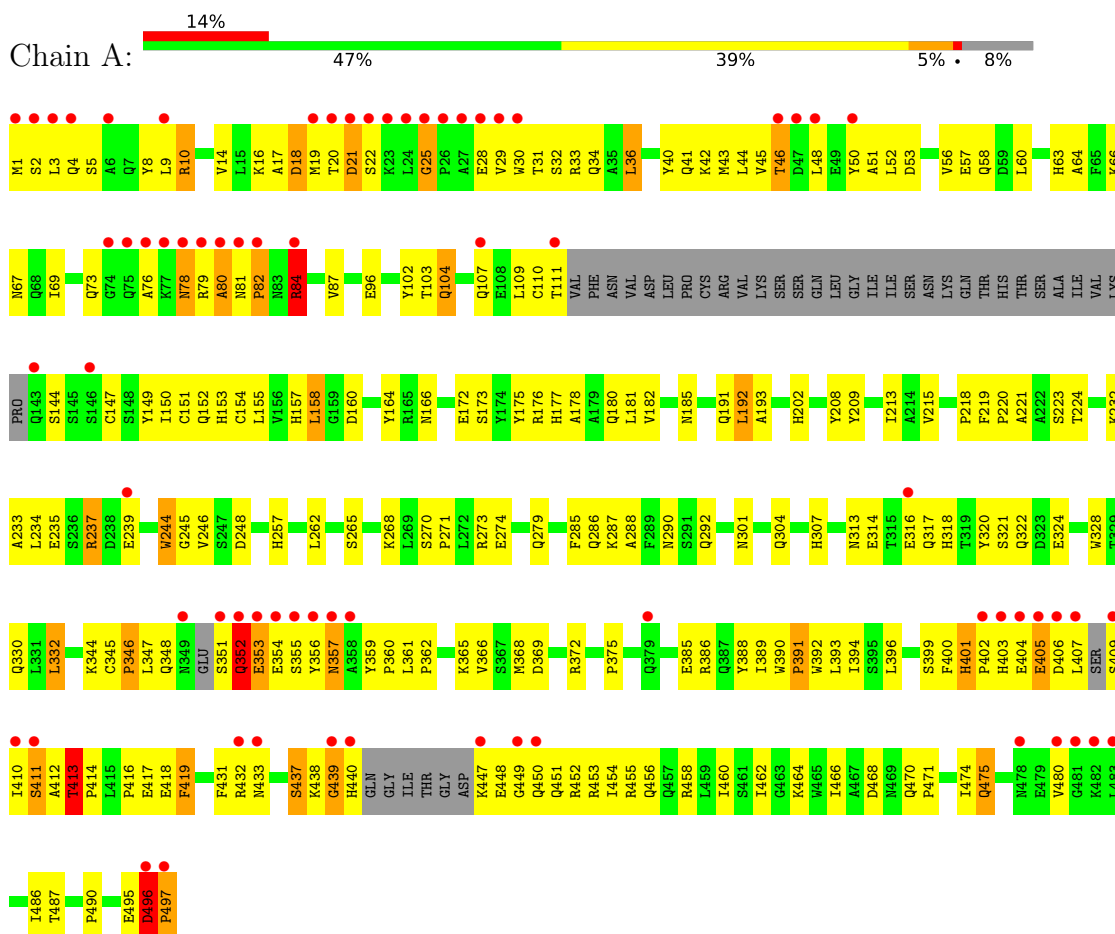
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	131	Total 131	O 131	0	0
3	B	188	Total 188	O 188	0	0

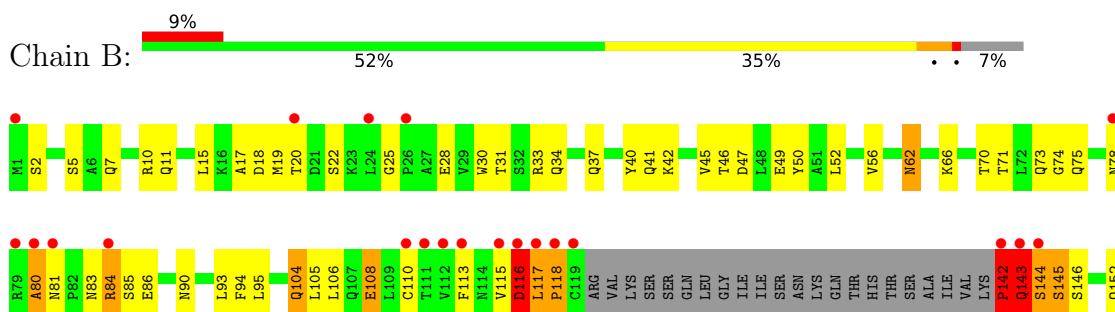
3 Residue-property plots

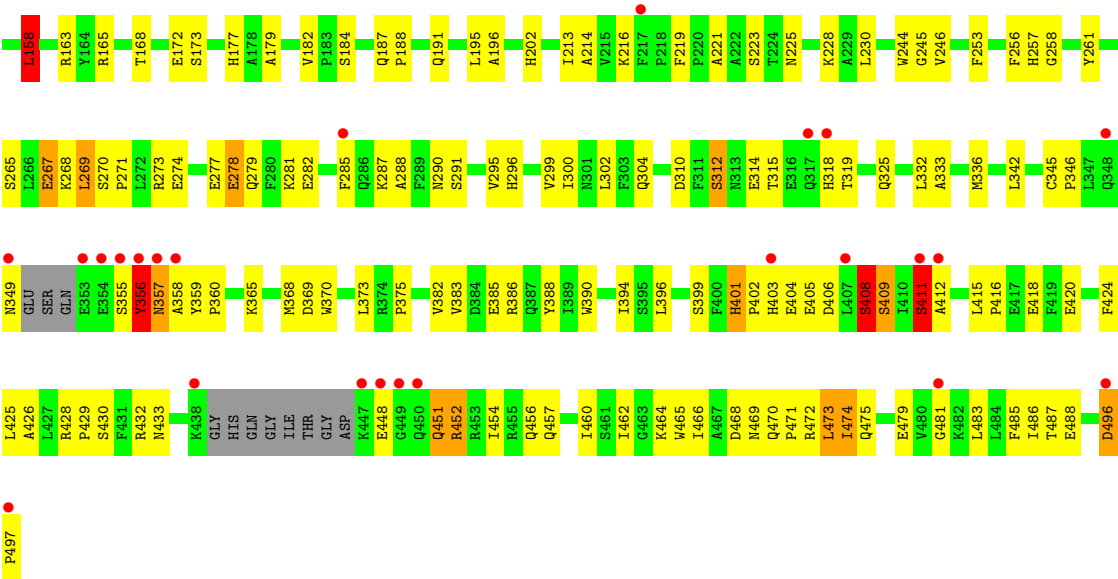
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: SMG-7 transcript variant 2



• Molecule 1: SMG-7 transcript variant 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.02Å 100.05Å 208.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.55 30.00 – 2.55	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.55) 99.3 (30.00-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.19 (at 2.54Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.246 , 0.287 0.249 , 0.290	Depositor DCC
R_{free} test set	2219 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	41.0	Xtriage
Anisotropy	0.416	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7854	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% 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

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.52	1/3820 (0.0%)	1.07	30/5165 (0.6%)
1	B	0.72	6/3869 (0.2%)	1.22	33/5236 (0.6%)
All	All	0.63	7/7689 (0.1%)	1.15	63/10401 (0.6%)

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	A	0	1
1	B	0	5
All	All	0	6

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	411	SER	C-N	-22.79	1.01	1.33
1	B	408	SER	C-N	-17.24	1.11	1.33
1	B	356	TYR	C-N	-10.30	1.19	1.33
1	B	409	SER	C-N	-10.21	1.19	1.33
1	B	357	ASN	C-N	-8.62	1.21	1.33
1	A	357	ASN	N-CA	-6.01	1.37	1.45
1	B	142	PRO	C-N	-5.52	1.25	1.33

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	411	SER	O-C-N	-21.98	93.35	122.59
1	B	411	SER	CA-C-N	20.68	161.04	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	411	SER	C-N-CA	20.68	161.04	121.54
1	B	408	SER	O-C-N	-17.15	99.78	122.59
1	B	408	SER	CA-C-N	16.58	149.07	122.21
1	B	408	SER	C-N-CA	16.58	149.07	122.21
1	B	409	SER	O-C-N	-15.65	104.23	123.17
1	B	451	GLN	N-CA-C	-12.19	97.88	113.72
1	A	28	GLU	N-CA-C	-11.24	97.55	114.64
1	A	78	ASN	CA-C-N	10.86	138.88	121.08
1	A	78	ASN	C-N-CA	10.86	138.88	121.08
1	A	496	ASP	N-CA-C	9.95	131.79	109.81
1	A	352	GLN	OE1-CD-NE2	-9.83	112.77	122.60
1	A	317	GLN	OE1-CD-NE2	-9.76	112.84	122.60
1	B	143	GLN	OE1-CD-NE2	-9.76	112.84	122.60
1	B	80	ALA	N-CA-C	-8.27	93.19	110.80
1	B	117	LEU	CA-C-N	8.24	130.15	119.84
1	B	117	LEU	C-N-CA	8.24	130.15	119.84
1	B	470	GLN	CA-C-N	8.18	127.75	119.24
1	B	470	GLN	C-N-CA	8.18	127.75	119.24
1	B	409	SER	CA-C-N	7.99	133.97	123.11
1	B	409	SER	C-N-CA	7.99	133.97	123.11
1	B	145	SER	N-CA-C	-7.98	104.06	113.88
1	B	357	ASN	O-C-N	7.93	133.74	123.11
1	A	80	ALA	N-CA-C	-7.84	100.42	111.24
1	B	269	LEU	N-CA-C	7.38	120.03	111.02
1	A	84	ARG	O-C-N	-7.36	113.30	122.35
1	B	143	GLN	CG-CD-NE2	7.28	127.31	116.40
1	B	158	LEU	N-CA-C	-7.25	103.38	111.28
1	B	356	TYR	O-C-N	7.24	130.69	122.22
1	B	62	ASN	N-CA-C	7.19	118.77	111.07
1	A	202	HIS	N-CA-C	7.10	118.66	111.07
1	B	454	ILE	N-CA-C	-6.72	103.94	110.72
1	A	21	ASP	CA-C-N	6.67	133.47	121.92
1	A	21	ASP	C-N-CA	6.67	133.47	121.92
1	A	352	GLN	CG-CD-NE2	6.66	126.39	116.40
1	A	317	GLN	CG-CD-NE2	6.64	126.36	116.40
1	A	158	LEU	N-CA-C	-6.55	104.39	112.38
1	A	356	TYR	N-CA-C	-6.31	104.50	111.82
1	B	17	ALA	N-CA-C	-6.24	104.02	111.69
1	A	20	THR	N-CA-C	-6.06	106.02	113.41
1	B	401	HIS	CA-C-N	6.02	126.05	119.90
1	B	401	HIS	C-N-CA	6.02	126.05	119.90
1	A	405	GLU	N-CA-C	-6.00	106.50	113.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	245	GLY	N-CA-C	-5.76	102.66	112.51
1	B	287	LYS	N-CA-C	5.59	119.14	111.54
1	A	22	SER	N-CA-C	-5.50	106.73	113.50
1	A	209	TYR	N-CA-C	-5.44	105.43	111.36
1	B	245	GLY	N-CA-C	-5.30	103.44	112.51
1	A	29	VAL	N-CA-C	-5.24	105.29	111.00
1	A	413	THR	CA-C-N	5.22	125.14	119.76
1	A	413	THR	C-N-CA	5.22	125.14	119.76
1	B	290	ASN	N-CA-C	-5.21	102.75	110.46
1	A	401	HIS	CA-C-N	5.18	125.19	119.90
1	A	401	HIS	C-N-CA	5.18	125.19	119.90
1	A	244	TRP	N-CA-C	5.15	118.46	110.17
1	A	10	ARG	N-CA-C	-5.10	105.72	111.28
1	A	403	HIS	N-CA-C	-5.08	101.06	108.07
1	A	21	ASP	O-C-N	5.07	129.33	122.59
1	B	202	HIS	N-CA-C	5.07	116.49	111.07
1	A	25	GLY	N-CA-C	5.04	122.61	112.34
1	B	415	LEU	N-CA-C	-5.03	103.81	110.40
1	B	488	GLU	N-CA-C	-5.01	107.17	113.28

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	84	ARG	Mainchain
1	B	408	SER	Peptide,Mainchain
1	B	409	SER	Peptide,Mainchain
1	B	411	SER	Peptide

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	3737	0	3697	190	0
1	B	3783	0	3745	172	0
2	A	5	0	0	0	0
2	B	10	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	131	0	0	20	0
3	B	188	0	0	32	0
All	All	7854	0	7442	360	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 25.

All (360) 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:B:349:ASN:HB2	1:B:356:TYR:CD1	1.78	1.18
1:B:349:ASN:HB2	1:B:356:TYR:HD1	1.03	1.11
1:A:81:ASN:HB3	1:A:84:ARG:HB3	1.22	1.11
1:B:257:HIS:HD2	1:B:304:GLN:HG3	0.98	1.07
1:B:257:HIS:CD2	1:B:304:GLN:HG3	1.91	1.05
1:B:93:LEU:HB2	3:B:648:HOH:O	1.59	1.01
1:A:81:ASN:CB	1:A:84:ARG:HB3	1.92	1.00
1:A:475:GLN:NE2	1:A:487:THR:HA	1.81	0.95
1:A:475:GLN:HE21	1:A:487:THR:HA	1.31	0.95
1:B:33:ARG:HH21	1:B:37:GLN:HE22	1.07	0.94
1:B:472:ARG:HB2	3:B:639:HOH:O	1.67	0.93
1:A:354:GLU:O	1:A:357:ASN:OD1	1.89	0.90
1:B:33:ARG:HE	1:B:37:GLN:NE2	1.71	0.89
1:A:405:GLU:C	1:A:407:LEU:H	1.81	0.88
1:A:344:LYS:HE3	1:A:348:GLN:HE21	1.38	0.88
1:A:257:HIS:ND1	1:A:304:GLN:HG3	1.88	0.87
1:A:344:LYS:HE3	1:A:348:GLN:NE2	1.89	0.87
1:A:351:SER:O	1:A:353:GLU:N	2.08	0.86
1:B:143:GLN:O	1:B:144:SER:HB3	1.77	0.85
1:A:19:MET:HE1	1:A:33:ARG:HB2	1.59	0.84
1:A:448:GLU:HG3	1:A:449:GLY:H	1.42	0.83
1:A:352:GLN:HB2	1:A:355:SER:HB3	1.59	0.83
1:A:447:LYS:O	1:A:451:GLN:HG3	1.80	0.82
1:B:333:ALA:HB2	1:B:382:VAL:HG11	1.61	0.81
1:A:69:ILE:O	1:A:73:GLN:HG3	1.80	0.81
1:A:475:GLN:HG2	1:A:486:ILE:HG13	1.64	0.80
1:B:172:GLU:HG2	1:B:195:LEU:HD23	1.62	0.80
1:B:71:THR:C	3:B:517:HOH:O	2.24	0.80
1:B:270:SER:HB3	1:B:271:PRO:HD3	1.64	0.79
1:B:300:ILE:HD12	3:B:536:HOH:O	1.81	0.79
1:A:110:CYS:HB3	1:A:151:CYS:SG	2.23	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:ARG:NH2	1:B:37:GLN:HE22	1.78	0.79
1:A:480:VAL:HG12	1:A:480:VAL:O	1.81	0.78
1:B:261:TYR:HB2	1:B:304:GLN:HE22	1.46	0.78
1:B:404:GLU:OE1	1:B:481:GLY:HA2	1.83	0.78
1:B:143:GLN:O	1:B:144:SER:CB	2.33	0.77
1:B:33:ARG:HE	1:B:37:GLN:HE21	1.30	0.77
1:B:74:GLY:N	3:B:517:HOH:O	2.17	0.77
1:B:365:LYS:HE3	1:B:369:ASP:OD2	1.86	0.76
1:B:246:VAL:HG22	1:B:288:ALA:HB1	1.68	0.74
1:B:452:ARG:O	1:B:456:GLN:HG3	1.86	0.74
1:A:60:LEU:O	1:A:64:ALA:HB3	1.87	0.73
1:A:180:GLN:HG2	3:A:617:HOH:O	1.88	0.73
1:A:153:HIS:ND1	3:A:502:HOH:O	2.22	0.72
1:A:404:GLU:HA	1:A:404:GLU:OE1	1.89	0.72
1:A:10:ARG:O	1:A:14:VAL:HG23	1.89	0.72
1:B:214:ALA:O	1:B:425:LEU:HG	1.89	0.72
1:A:359:TYR:N	1:A:360:PRO:CD	2.53	0.72
1:B:2:SER:HA	3:B:558:HOH:O	1.89	0.72
1:A:30:TRP:CZ3	1:A:33:ARG:HD3	2.25	0.71
1:B:406:ASP:HA	1:B:457:GLN:HE21	1.55	0.71
1:B:403:HIS:HB3	3:B:664:HOH:O	1.91	0.71
1:A:407:LEU:C	1:A:409:SER:HB3	2.15	0.70
1:A:31:THR:O	3:A:501:HOH:O	2.10	0.70
1:B:310:ASP:OD2	1:B:312:SER:HB3	1.90	0.70
1:A:285:PHE:HE2	1:A:348:GLN:NE2	1.91	0.69
1:B:117:LEU:HD12	1:B:118:PRO:HD2	1.74	0.69
1:A:452:ARG:O	1:A:456:GLN:HG3	1.93	0.69
1:A:405:GLU:O	1:A:407:LEU:N	2.26	0.68
1:A:359:TYR:CD2	1:A:360:PRO:HD3	2.28	0.67
1:A:185:ASN:HB3	3:A:535:HOH:O	1.94	0.67
1:A:410:ILE:O	1:A:412:ALA:N	2.27	0.67
1:A:172:GLU:O	1:A:176:ARG:HG2	1.94	0.67
1:B:278:GLU:HG3	1:B:279:GLN:N	2.08	0.67
1:A:322:GLN:HB3	3:A:592:HOH:O	1.96	0.66
1:A:401:HIS:N	1:A:402:PRO:HD3	2.10	0.66
1:A:359:TYR:H	1:A:360:PRO:HD3	1.62	0.65
1:A:365:LYS:HD3	1:A:369:ASP:OD2	1.95	0.65
1:A:344:LYS:CE	1:A:348:GLN:HE21	2.08	0.65
1:A:344:LYS:HD2	1:A:392:TRP:CE2	2.32	0.65
1:B:19:MET:CE	1:B:33:ARG:HG3	2.26	0.65
1:A:109:LEU:HD13	1:A:150:ILE:HD13	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ALA:HB2	1:A:87:VAL:HG12	1.79	0.65
1:A:107:GLN:O	1:A:111:THR:HB	1.97	0.65
1:B:368:MET:HB3	1:B:462:ILE:HG21	1.79	0.64
1:B:486:ILE:CG2	1:B:487:THR:N	2.60	0.64
1:B:349:ASN:HB2	1:B:356:TYR:CE1	2.33	0.64
1:A:344:LYS:CE	1:A:348:GLN:NE2	2.61	0.63
1:A:456:GLN:O	1:A:460:ILE:HG12	1.98	0.63
1:B:62:ASN:HA	1:B:66:LYS:HB3	1.81	0.63
1:A:394:ILE:CD1	1:A:487:THR:HB	2.29	0.62
1:A:416:PRO:HD2	3:A:563:HOH:O	1.99	0.62
1:B:416:PRO:HG2	1:B:451:GLN:HE22	1.65	0.62
1:B:19:MET:HE1	1:B:33:ARG:HG3	1.80	0.62
1:A:173:SER:O	1:A:177:HIS:HD2	1.82	0.62
1:A:270:SER:HB3	1:A:271:PRO:HD3	1.81	0.62
1:A:314:GLU:OE1	1:A:375:PRO:HD2	2.00	0.61
1:A:63:HIS:HA	1:A:67:ASN:ND2	2.15	0.61
1:B:382:VAL:HG13	1:B:386:ARG:NH1	2.15	0.61
1:A:361:LEU:HB3	1:A:455:ARG:HD2	1.82	0.61
1:A:18:ASP:O	1:A:21:ASP:HB2	1.98	0.61
1:A:102:TYR:HB2	1:A:158:LEU:HD13	1.83	0.61
1:A:448:GLU:O	1:A:451:GLN:N	2.28	0.61
1:A:16:LYS:HD3	1:A:63:HIS:CE1	2.36	0.60
1:A:344:LYS:HD2	1:A:392:TRP:CZ2	2.36	0.60
1:B:401:HIS:N	1:B:402:PRO:HD3	2.17	0.60
1:B:333:ALA:CB	1:B:382:VAL:HG11	2.31	0.60
1:A:5:SER:HB3	1:A:50:TYR:CD2	2.35	0.60
1:B:315:THR:O	1:B:315:THR:HG22	2.00	0.60
1:A:44:LEU:HD22	1:A:150:ILE:HD12	1.84	0.59
1:A:34:GLN:N	3:A:501:HOH:O	2.35	0.59
1:B:318:HIS:CD2	1:B:319:THR:H	2.20	0.59
1:A:359:TYR:N	1:A:360:PRO:HD3	2.17	0.59
1:B:281:LYS:O	1:B:285:PHE:HD1	1.86	0.59
1:B:110:CYS:SG	1:B:117:LEU:HD23	2.43	0.59
1:B:474:ILE:HD11	1:B:485:PHE:HD2	1.68	0.59
1:B:318:HIS:HD2	1:B:319:THR:H	1.51	0.59
1:A:285:PHE:CE2	1:A:348:GLN:NE2	2.70	0.58
1:A:32:SER:C	3:A:501:HOH:O	2.46	0.58
1:A:344:LYS:HG3	1:A:392:TRP:CD2	2.39	0.58
1:A:365:LYS:HZ1	1:A:418:GLU:HG2	1.67	0.58
1:B:196:ALA:HA	3:B:579:HOH:O	2.04	0.58
1:B:265:SER:HA	1:B:267:GLU:OE2	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:GLN:O	1:B:460:ILE:HG12	2.03	0.58
1:A:273:ARG:NH2	1:A:274:GLU:OE2	2.35	0.58
1:B:465:TRP:CE3	1:B:466:ILE:HD13	2.39	0.58
1:A:48:LEU:O	1:A:52:LEU:HD13	2.04	0.58
1:B:191:GLN:NE2	3:B:671:HOH:O	2.30	0.58
1:B:33:ARG:NE	1:B:37:GLN:NE2	2.47	0.58
1:B:219:PHE:CE2	1:B:221:ALA:HB3	2.39	0.57
1:B:382:VAL:HG13	1:B:386:ARG:HH12	1.68	0.57
1:A:57:GLU:HG3	1:A:58:GLN:HG3	1.86	0.57
1:A:410:ILE:C	1:A:412:ALA:N	2.62	0.57
1:B:349:ASN:CB	1:B:356:TYR:CD1	2.72	0.57
1:B:465:TRP:HE3	1:B:466:ILE:HD13	1.68	0.57
1:A:405:GLU:C	1:A:407:LEU:N	2.50	0.57
1:A:416:PRO:HD3	1:A:451:GLN:NE2	2.19	0.57
1:B:496:ASP:HB3	1:B:497:PRO:CD	2.34	0.57
1:A:285:PHE:HE2	1:A:348:GLN:HE22	1.51	0.57
1:B:33:ARG:NE	3:B:568:HOH:O	2.38	0.57
1:A:345:CYS:HB3	1:A:346:PRO:HD3	1.86	0.57
1:B:173:SER:O	1:B:177:HIS:HD2	1.88	0.57
1:B:345:CYS:HB3	1:B:346:PRO:HD3	1.85	0.56
1:A:359:TYR:O	3:A:525:HOH:O	2.18	0.56
1:B:31:THR:HG22	3:B:510:HOH:O	2.03	0.56
1:B:282:GLU:CD	3:B:601:HOH:O	2.48	0.56
1:B:113:PHE:O	1:B:115:VAL:HG23	2.06	0.56
1:B:486:ILE:HG22	1:B:487:THR:N	2.19	0.56
1:B:214:ALA:C	1:B:425:LEU:HG	2.30	0.56
1:A:313:ASN:ND2	1:A:320:TYR:OH	2.39	0.56
1:A:219:PHE:CE2	1:A:221:ALA:HB3	2.40	0.56
1:A:480:VAL:O	1:A:480:VAL:CG1	2.54	0.55
1:A:42:LYS:O	1:A:46:THR:HB	2.07	0.55
1:A:347:LEU:HD12	3:A:554:HOH:O	2.05	0.55
1:A:414:PRO:HB2	1:A:419:PHE:CD1	2.41	0.55
1:B:349:ASN:CB	1:B:356:TYR:HD1	1.97	0.55
1:A:63:HIS:HA	1:A:67:ASN:HD22	1.72	0.55
1:B:359:TYR:CG	1:B:360:PRO:HD3	2.42	0.55
1:B:356:TYR:N	1:B:356:TYR:CD2	2.75	0.55
1:B:7:GLN:O	1:B:11:GLN:HG3	2.07	0.55
1:A:496:ASP:O	1:A:497:PRO:O	2.25	0.55
1:B:40:TYR:CD2	1:B:56:VAL:HG13	2.42	0.54
1:B:253:PHE:CZ	1:B:257:HIS:HE1	2.24	0.54
1:B:296:HIS:C	3:B:536:HOH:O	2.50	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:GLU:HG3	1:A:58:GLN:N	2.21	0.54
1:A:439:GLY:O	1:A:440:HIS:HB2	2.07	0.54
1:B:432:ARG:HG3	1:B:433:ASN:N	2.22	0.54
1:B:428:ARG:HB2	1:B:429:PRO:HD3	1.89	0.53
1:B:71:THR:O	1:B:75:GLN:HG3	2.07	0.53
1:A:40:TYR:CD2	1:A:56:VAL:HG13	2.43	0.53
1:A:17:ALA:N	3:A:499:HOH:O	2.41	0.53
1:A:232:LYS:O	1:A:235:GLU:HB2	2.09	0.53
1:A:368:MET:HB3	1:A:462:ILE:HG21	1.90	0.53
1:B:81:ASN:HD22	1:B:84:ARG:N	2.06	0.53
1:A:365:LYS:NZ	1:A:418:GLU:HG2	2.24	0.53
1:B:172:GLU:HB3	3:B:650:HOH:O	2.09	0.53
1:A:36:LEU:HD22	1:A:40:TYR:CE1	2.45	0.52
1:A:410:ILE:O	1:A:411:SER:C	2.51	0.52
1:A:431:PHE:O	1:A:433:ASN:N	2.40	0.52
1:B:33:ARG:CZ	3:B:568:HOH:O	2.56	0.52
1:B:273:ARG:NH2	1:B:274:GLU:OE2	2.42	0.52
1:A:237:ARG:NH1	1:A:268:LYS:NZ	2.58	0.52
1:B:416:PRO:HG2	1:B:451:GLN:NE2	2.24	0.52
1:B:115:VAL:C	1:B:117:LEU:H	2.17	0.52
1:B:267:GLU:CD	1:B:267:GLU:H	2.17	0.52
1:B:382:VAL:CG1	1:B:386:ARG:NH1	2.71	0.52
1:B:475:GLN:HA	3:B:665:HOH:O	2.08	0.52
1:A:286:GLN:O	1:A:287:LYS:HB2	2.09	0.52
1:B:116:ASP:O	1:B:117:LEU:C	2.52	0.52
1:A:246:VAL:CG2	1:A:288:ALA:HB1	2.40	0.52
1:A:448:GLU:HG3	1:A:449:GLY:N	2.17	0.52
1:A:353:GLU:O	1:A:354:GLU:HB2	2.08	0.52
1:A:44:LEU:HD22	1:A:150:ILE:CD1	2.40	0.52
1:B:163:ARG:NH2	2:B:498:SO4:O1	2.43	0.52
1:B:253:PHE:CZ	1:B:257:HIS:CE1	2.98	0.52
1:A:40:TYR:HD2	1:A:43:MET:CE	2.22	0.51
1:A:321:SER:HB3	1:A:324:GLU:HG3	1.91	0.51
1:B:33:ARG:NH1	1:B:94:PHE:CE2	2.78	0.51
1:A:4:GLN:HG3	1:A:8:TYR:CE1	2.45	0.51
1:B:244:TRP:CD2	1:B:279:GLN:HG3	2.46	0.51
1:B:273:ARG:HD2	1:B:333:ALA:HB3	1.93	0.51
1:A:396:LEU:O	1:A:399:SER:HB3	2.10	0.50
1:A:411:SER:C	1:A:413:THR:H	2.20	0.50
1:A:414:PRO:HB2	1:A:419:PHE:HD1	1.76	0.50
1:B:187:GLN:HB3	1:B:188:PRO:HD3	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:LYS:O	1:B:271:PRO:HD2	2.11	0.50
1:A:180:GLN:NE2	3:A:616:HOH:O	2.43	0.50
1:B:47:ASP:HB3	3:B:509:HOH:O	2.11	0.50
1:A:307:HIS:HE1	3:A:620:HOH:O	1.95	0.50
1:B:356:TYR:N	1:B:356:TYR:HD2	2.09	0.50
1:B:355:SER:O	1:B:359:TYR:CD2	2.66	0.49
1:B:93:LEU:HD23	3:B:636:HOH:O	2.12	0.49
1:A:417:GLU:OE2	1:A:455:ARG:NH1	2.46	0.49
1:A:144:SER:HB3	1:A:147:CYS:HB2	1.93	0.49
1:B:146:SER:HB2	3:B:679:HOH:O	2.13	0.49
1:A:102:TYR:CB	1:A:158:LEU:HD13	2.43	0.49
1:A:218:PRO:O	1:A:220:PRO:HD3	2.13	0.48
1:A:239:GLU:HG3	3:A:586:HOH:O	2.13	0.48
1:A:394:ILE:HD13	1:A:487:THR:HB	1.95	0.48
1:B:45:VAL:HG21	1:B:108:GLU:OE1	2.13	0.48
1:A:359:TYR:H	1:A:360:PRO:CD	2.20	0.48
1:B:78:ASN:O	1:B:80:ALA:N	2.45	0.48
1:B:152:GLN:NE2	1:B:182:VAL:HB	2.28	0.48
1:A:18:ASP:N	3:A:499:HOH:O	2.46	0.48
1:A:79:ARG:O	1:A:80:ALA:C	2.56	0.48
1:B:106:LEU:HD21	1:B:117:LEU:HD21	1.96	0.48
1:A:57:GLU:OE1	1:A:149:TYR:HE2	1.96	0.48
1:A:257:HIS:HE2	1:A:301:ASN:ND2	2.12	0.48
1:B:281:LYS:O	1:B:285:PHE:CD1	2.66	0.48
1:A:175:TYR:CZ	1:A:191:GLN:HB3	2.48	0.47
1:A:244:TRP:HB3	1:A:248:ASP:HB2	1.96	0.47
1:B:90:ASN:O	3:B:648:HOH:O	2.20	0.47
1:A:40:TYR:HD2	1:A:43:MET:HE3	1.78	0.47
1:B:221:ALA:O	1:B:225:ASN:ND2	2.47	0.47
1:A:182:VAL:HG11	1:A:185:ASN:ND2	2.29	0.47
1:A:400:PHE:HD1	1:A:460:ILE:HD11	1.78	0.47
1:A:1:MET:C	1:A:3:LEU:H	2.23	0.47
1:A:316:GLU:HG3	1:A:318:HIS:CE1	2.50	0.47
1:B:216:LYS:HG2	3:B:581:HOH:O	2.14	0.47
1:B:448:GLU:O	1:B:451:GLN:HG2	2.15	0.47
1:A:313:ASN:HD22	1:A:318:HIS:HD2	1.61	0.47
1:B:10:ARG:NH2	3:B:561:HOH:O	2.43	0.47
1:A:79:ARG:O	1:A:80:ALA:HB3	2.15	0.47
1:A:449:GLY:O	1:A:453:ARG:HB2	2.15	0.47
1:B:33:ARG:NH1	1:B:94:PHE:HE2	2.13	0.47
1:A:268:LYS:O	1:A:271:PRO:HD2	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:HIS:N	1:A:402:PRO:CD	2.77	0.46
1:B:5:SER:HB3	1:B:50:TYR:CD2	2.50	0.46
1:A:405:GLU:HA	1:A:407:LEU:CD1	2.45	0.46
1:A:455:ARG:NH1	1:A:455:ARG:HB2	2.31	0.46
1:A:232:LYS:HA	1:A:235:GLU:OE2	2.16	0.46
1:A:388:TYR:O	1:A:391:PRO:HD2	2.16	0.46
1:A:412:ALA:O	1:A:414:PRO:HD3	2.16	0.46
1:B:41:GLN:HG3	1:B:105:LEU:CD1	2.46	0.46
1:A:257:HIS:CE1	1:A:301:ASN:HD22	2.32	0.46
1:B:396:LEU:O	1:B:399:SER:HB3	2.16	0.46
1:B:359:TYR:N	1:B:360:PRO:CD	2.79	0.46
3:A:602:HOH:O	1:B:267:GLU:HG2	2.15	0.45
1:B:357:ASN:O	1:B:358:ALA:HB3	2.16	0.45
1:B:405:GLU:HA	1:B:408:SER:OG	2.17	0.45
1:A:31:THR:C	3:A:501:HOH:O	2.55	0.45
1:B:342:LEU:O	1:B:346:PRO:HD3	2.17	0.45
1:A:455:ARG:NH2	3:A:563:HOH:O	2.45	0.45
1:A:1:MET:C	1:A:3:LEU:N	2.73	0.45
1:A:215:VAL:O	1:A:218:PRO:HD3	2.17	0.45
1:A:362:PRO:O	1:A:366:VAL:HG23	2.16	0.45
1:A:437:SER:OG	1:A:438:LYS:N	2.48	0.45
1:A:1:MET:O	1:A:3:LEU:N	2.49	0.45
1:B:230:LEU:HD13	1:B:258:GLY:HA2	1.97	0.45
1:A:81:ASN:O	1:A:82:PRO:C	2.60	0.44
1:A:173:SER:O	1:A:177:HIS:CD2	2.66	0.44
1:B:95:LEU:HD13	1:B:165:ARG:HG3	1.99	0.44
1:B:314:GLU:HB3	3:B:607:HOH:O	2.17	0.44
1:A:496:ASP:O	1:A:497:PRO:C	2.59	0.44
1:A:290:ASN:OD1	1:A:292:GLN:HB3	2.16	0.44
1:A:490:PRO:HD2	1:B:271:PRO:HG2	2.00	0.44
1:B:253:PHE:CE1	1:B:257:HIS:HE1	2.35	0.44
1:B:291:SER:HB3	1:B:359:TYR:HA	2.00	0.44
1:A:474:ILE:HG22	1:A:475:GLN:N	2.33	0.44
1:B:168:THR:O	1:B:172:GLU:HG3	2.17	0.44
1:B:256:PHE:CE1	1:B:269:LEU:HD22	2.52	0.44
1:A:352:GLN:O	1:A:353:GLU:C	2.61	0.44
1:A:372:ARG:HD3	3:A:532:HOH:O	2.17	0.44
1:B:424:PHE:O	1:B:428:ARG:HG3	2.17	0.44
1:A:385:GLU:OE2	1:B:385:GLU:OE1	2.36	0.44
1:A:458:ARG:O	1:A:462:ILE:HG13	2.18	0.44
1:B:142:PRO:HB2	1:B:143:GLN:H	1.26	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:ILE:C	1:A:412:ALA:H	2.24	0.44
1:A:103:THR:O	1:A:107:GLN:HG3	2.17	0.43
1:A:154:CYS:O	1:A:158:LEU:HB2	2.17	0.43
1:A:234:LEU:HD12	1:A:262:LEU:HD12	1.99	0.43
1:B:390:TRP:O	1:B:394:ILE:HD13	2.18	0.43
1:B:497:PRO:HB3	3:B:668:HOH:O	2.18	0.43
1:B:30:TRP:O	1:B:34:GLN:HG2	2.18	0.43
1:B:277:GLU:OE1	3:B:656:HOH:O	2.20	0.43
1:A:152:GLN:HG3	1:A:178:ALA:O	2.19	0.43
1:A:316:GLU:H	1:A:316:GLU:HG2	1.63	0.43
1:A:359:TYR:CG	1:A:360:PRO:HD3	2.54	0.43
1:B:33:ARG:CZ	1:B:37:GLN:HE22	2.31	0.43
1:B:172:GLU:CG	1:B:195:LEU:HD23	2.41	0.43
1:B:325:GLN:HG2	3:B:685:HOH:O	2.17	0.43
1:B:70:THR:O	3:B:517:HOH:O	2.21	0.43
1:B:83:ASN:O	1:B:84:ARG:C	2.62	0.43
1:B:302:LEU:HD22	1:B:370:TRP:CG	2.54	0.43
1:A:466:ILE:HG21	1:A:474:ILE:HD12	2.00	0.43
1:B:25:GLY:O	1:B:28:GLU:HB2	2.18	0.43
1:A:386:ARG:C	1:A:388:TYR:H	2.27	0.42
1:B:158:LEU:HD12	1:B:158:LEU:HA	1.87	0.42
1:B:390:TRP:CD1	1:B:473:LEU:HG	2.54	0.42
1:B:474:ILE:CD1	1:B:485:PHE:HD2	2.32	0.42
1:A:41:GLN:HE22	1:A:104:GLN:CD	2.27	0.42
1:B:464:LYS:HE3	1:B:468:ASP:OD2	2.20	0.42
1:B:469:ASN:C	1:B:471:PRO:HD3	2.44	0.42
1:B:104:GLN:HE21	1:B:104:GLN:HB3	1.68	0.42
1:A:273:ARG:HD3	1:A:330:GLN:OE1	2.19	0.42
1:A:450:GLN:O	1:A:454:ILE:HG13	2.19	0.42
1:B:83:ASN:O	1:B:86:GLU:HG2	2.19	0.42
1:A:244:TRP:CD2	1:A:279:GLN:HG3	2.54	0.42
1:B:33:ARG:HH11	1:B:94:PHE:HE2	1.67	0.42
1:B:219:PHE:HE2	1:B:221:ALA:HB3	1.83	0.42
1:B:402:PRO:HB2	1:B:483:LEU:HB2	2.01	0.42
1:A:57:GLU:CG	1:A:58:GLN:N	2.83	0.42
1:A:464:LYS:HD2	1:A:468:ASP:OD2	2.20	0.42
1:A:157:HIS:HD2	1:A:160:ASP:OD2	2.02	0.42
1:B:246:VAL:CG2	1:B:288:ALA:HB1	2.45	0.42
1:B:420:GLU:HB3	3:B:626:HOH:O	2.19	0.42
1:B:355:SER:O	1:B:359:TYR:CE2	2.72	0.42
1:A:155:LEU:HD12	1:A:181:LEU:HD12	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:LEU:O	1:A:396:LEU:HB3	2.20	0.41
1:B:15:LEU:O	1:B:18:ASP:HB2	2.20	0.41
1:B:20:THR:HG22	1:B:20:THR:O	2.20	0.41
1:A:8:TYR:CZ	1:A:42:LYS:HE3	2.55	0.41
1:A:448:GLU:O	1:A:449:GLY:C	2.61	0.41
1:B:49:GLU:HB2	3:B:559:HOH:O	2.20	0.41
1:B:15:LEU:HD23	1:B:15:LEU:HA	1.89	0.41
1:B:52:LEU:HD23	1:B:52:LEU:HA	1.90	0.41
1:B:83:ASN:O	1:B:85:SER:N	2.53	0.41
1:B:336:MET:HG3	1:B:383:VAL:HG22	2.02	0.41
1:B:370:TRP:CD1	1:B:426:ALA:HB1	2.55	0.41
1:A:213:ILE:HD11	1:A:223:SER:HA	2.02	0.41
1:A:389:ILE:HG13	1:A:390:TRP:N	2.34	0.41
1:A:495:GLU:O	1:A:497:PRO:HD2	2.20	0.41
1:B:388:TYR:CD1	1:B:388:TYR:C	2.98	0.41
1:A:455:ARG:NH1	3:A:563:HOH:O	2.47	0.41
1:B:295:VAL:O	1:B:299:VAL:HG23	2.20	0.41
1:A:51:ALA:O	1:A:56:VAL:HG23	2.21	0.41
1:A:66:LYS:HE2	1:A:164:TYR:OH	2.20	0.41
1:A:233:ALA:C	1:A:235:GLU:H	2.28	0.41
1:B:394:ILE:HD11	1:B:474:ILE:HB	2.02	0.41
1:B:496:ASP:HB3	1:B:497:PRO:HD2	2.03	0.41
1:A:30:TRP:HZ3	1:A:33:ARG:HD3	1.81	0.41
1:A:417:GLU:OE1	1:A:417:GLU:N	2.48	0.41
1:A:448:GLU:C	1:A:450:GLN:N	2.78	0.41
1:B:30:TRP:CZ3	1:B:33:ARG:NH1	2.89	0.41
1:B:34:GLN:HG3	3:B:567:HOH:O	2.20	0.41
1:B:152:GLN:HE22	1:B:182:VAL:HB	1.86	0.41
1:B:213:ILE:HD11	1:B:223:SER:HA	2.03	0.41
1:A:175:TYR:HB3	1:A:192:LEU:HG	2.03	0.41
1:B:42:LYS:O	1:B:46:THR:HG23	2.21	0.41
1:B:73:GLN:N	3:B:517:HOH:O	2.53	0.41
1:B:179:ALA:HA	3:B:526:HOH:O	2.21	0.41
1:A:41:GLN:O	1:A:45:VAL:HG23	2.21	0.40
1:A:431:PHE:C	1:A:433:ASN:H	2.29	0.40
1:A:470:GLN:N	1:A:471:PRO:HD3	2.37	0.40
1:A:394:ILE:HD11	1:A:474:ILE:HG12	2.03	0.40
1:B:373:LEU:C	1:B:375:PRO:HD3	2.46	0.40
1:A:57:GLU:HG3	1:A:58:GLN:H	1.84	0.40
1:A:193:ALA:HB2	1:A:208:TYR:CB	2.51	0.40
1:B:365:LYS:NZ	1:B:418:GLU:HG3	2.37	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:TRP:O	1:A:332:LEU:HB2	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	448/497 (90%)	399 (89%)	36 (8%)	13 (3%)	3	3
1	B	456/497 (92%)	413 (91%)	33 (7%)	10 (2%)	5	5
All	All	904/994 (91%)	812 (90%)	69 (8%)	23 (2%)	4	4

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	352	GLN
1	A	411	SER
1	A	432	ARG
1	A	437	SER
1	B	84	ARG
1	B	118	PRO
1	B	412	ALA
1	A	496	ASP
1	B	22	SER
1	B	116	ASP
1	B	143	GLN
1	B	479	GLU
1	A	2	SER
1	A	353	GLU
1	A	406	ASP
1	A	25	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	82	PRO
1	A	439	GLY
1	B	144	SER
1	B	411	SER
1	A	346	PRO
1	B	496	ASP

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	412/447 (92%)	393 (95%)	19 (5%)	24	36
1	B	419/447 (94%)	402 (96%)	17 (4%)	27	41
All	All	831/894 (93%)	795 (96%)	36 (4%)	26	39

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	18	ASP
1	A	36	LEU
1	A	46	THR
1	A	53	ASP
1	A	96	GLU
1	A	104	GLN
1	A	166	ASN
1	A	192	LEU
1	A	224	THR
1	A	237	ARG
1	A	265	SER
1	A	332	LEU
1	A	391	PRO
1	A	413	THR
1	A	419	PHE
1	A	475	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	496	ASP
1	A	497	PRO
1	B	104	GLN
1	B	108	GLU
1	B	116	ASP
1	B	142	PRO
1	B	145	SER
1	B	158	LEU
1	B	184	SER
1	B	228	LYS
1	B	267	GLU
1	B	278	GLU
1	B	312	SER
1	B	332	LEU
1	B	356	TYR
1	B	430	SER
1	B	452	ARG
1	B	473	LEU
1	B	474	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	41	GLN
1	A	67	ASN
1	A	73	GLN
1	A	104	GLN
1	A	153	HIS
1	A	157	HIS
1	A	167	GLN
1	A	177	HIS
1	A	185	ASN
1	A	190	ASN
1	A	191	GLN
1	A	225	ASN
1	A	301	ASN
1	A	313	ASN
1	A	318	HIS
1	A	348	GLN
1	A	422	GLN
1	A	451	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	475	GLN
1	B	11	GLN
1	B	37	GLN
1	B	58	GLN
1	B	81	ASN
1	B	177	HIS
1	B	190	ASN
1	B	257	HIS
1	B	259	HIS
1	B	286	GLN
1	B	301	ASN
1	B	304	GLN
1	B	318	HIS
1	B	325	GLN
1	B	422	GLN
1	B	451	GLN
1	B	457	GLN
1	B	478	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	SO4	A	498	-	4,4,4	0.32	0	6,6,6	0.08	0
2	SO4	B	499	-	4,4,4	0.37	0	6,6,6	0.09	0
2	SO4	B	498	-	4,4,4	0.33	0	6,6,6	0.20	0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	498	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	409:SER	C	410:ILE	N	1.19
1	B	356:TYR	C	357:ASN	N	1.18
1	B	408:SER	C	409:SER	N	1.11
1	B	411:SER	C	412:ALA	N	1.01

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, 95th 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 ²)	Q<0.9
1	A	458/497 (92%)	0.78	71 (15%) 5 4	20, 43, 78, 91	54 (11%)
1	B	464/497 (93%)	0.42	45 (9%) 13 12	19, 36, 71, 106	30 (6%)
All	All	922/994 (92%)	0.60	116 (12%) 8 7	19, 40, 74, 106	84 (9%)

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	356	TYR	8.2
1	B	358	ALA	7.4
1	A	78	ASN	6.5
1	A	81	ASN	5.6
1	A	349	ASN	5.6
1	B	118	PRO	5.6
1	B	481	GLY	5.4
1	B	119	CYS	5.3
1	A	80	ALA	5.1
1	A	1	MET	4.8
1	A	409	SER	4.8
1	B	80	ALA	4.8
1	A	26	PRO	4.7
1	A	497	PRO	4.7
1	A	19	MET	4.6
1	B	142	PRO	4.6
1	A	358	ALA	4.5
1	B	411	SER	4.4
1	A	351	SER	4.2
1	A	407	LEU	4.2
1	A	22	SER	4.2
1	B	353	GLU	3.9
1	B	449	GLY	3.9
1	A	24	LEU	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	239	GLU	3.9
1	A	404	GLU	3.9
1	A	440	HIS	3.8
1	B	357	ASN	3.8
1	B	496	ASP	3.8
1	A	2	SER	3.7
1	A	480	VAL	3.7
1	B	79	ARG	3.7
1	A	405	GLU	3.7
1	A	449	GLY	3.7
1	A	23	LYS	3.7
1	A	84	ARG	3.6
1	A	481	GLY	3.6
1	A	439	GLY	3.5
1	A	3	LEU	3.5
1	A	25	GLY	3.5
1	A	482	LYS	3.5
1	A	410	ILE	3.4
1	B	450	GLN	3.4
1	A	353	GLU	3.3
1	A	50	TYR	3.3
1	B	143	GLN	3.2
1	B	349	ASN	3.2
1	A	411	SER	3.1
1	B	355	SER	3.1
1	A	496	ASP	3.1
1	A	75	GLN	3.1
1	A	406	ASP	3.1
1	B	84	ARG	3.1
1	A	356	TYR	3.0
1	B	81	ASN	3.0
1	A	79	ARG	3.0
1	A	82	PRO	3.0
1	A	77	LYS	2.9
1	B	111	THR	2.9
1	A	21	ASP	2.9
1	A	27	ALA	2.9
1	B	497	PRO	2.9
1	B	117	LEU	2.8
1	A	48	LEU	2.8
1	B	20	THR	2.8
1	A	450	GLN	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	348	GLN	2.8
1	A	483	LEU	2.7
1	A	403	HIS	2.7
1	B	448	GLU	2.7
1	A	6	ALA	2.7
1	B	407	LEU	2.7
1	B	354	GLU	2.6
1	A	316	GLU	2.6
1	B	115	VAL	2.6
1	B	113	PHE	2.6
1	B	24	LEU	2.6
1	B	403	HIS	2.6
1	A	46	THR	2.5
1	A	28	GLU	2.5
1	B	144	SER	2.5
1	B	1	MET	2.5
1	B	317	GLN	2.5
1	A	47	ASP	2.4
1	A	433	ASN	2.4
1	A	76	ALA	2.4
1	A	111	THR	2.3
1	A	402	PRO	2.3
1	B	26	PRO	2.3
1	A	4	GLN	2.3
1	B	116	ASP	2.3
1	B	285	PHE	2.3
1	B	438	LYS	2.3
1	A	352	GLN	2.3
1	A	355	SER	2.3
1	B	318	HIS	2.2
1	B	217	PHE	2.2
1	B	112	VAL	2.2
1	A	29	VAL	2.2
1	A	447	LYS	2.2
1	B	78	ASN	2.2
1	A	20	THR	2.2
1	B	447	LYS	2.2
1	A	478	ASN	2.1
1	A	107	GLN	2.1
1	A	357	ASN	2.1
1	A	9	LEU	2.1
1	A	379	GLN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	146	SER	2.1
1	B	110	CYS	2.1
1	A	143	GLN	2.1
1	B	412	ALA	2.0
1	A	30	TRP	2.0
1	A	74	GLY	2.0
1	A	432	ARG	2.0
1	A	354	GLU	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 oligosaccharides 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. The B-factors column lists the minimum, median, 95th 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	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	498	5/5	0.91	0.12	64,66,68,68	0
2	SO4	B	499	5/5	0.92	0.14	78,78,79,79	0
2	SO4	B	498	5/5	0.93	0.08	53,54,56,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.