



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:08 PM GMT

PDB ID : 1E7B
Title : CRYSTAL STRUCTURE OF HUMAN SERUM ALBUMIN COMPLEXED
WITH THE GENERAL ANESTHETIC HALOTHANE
Authors : Bhattacharya, A.A.; Curry, S.; Franks, N.P.
Deposited on : 2000-08-26
Resolution : 2.38 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

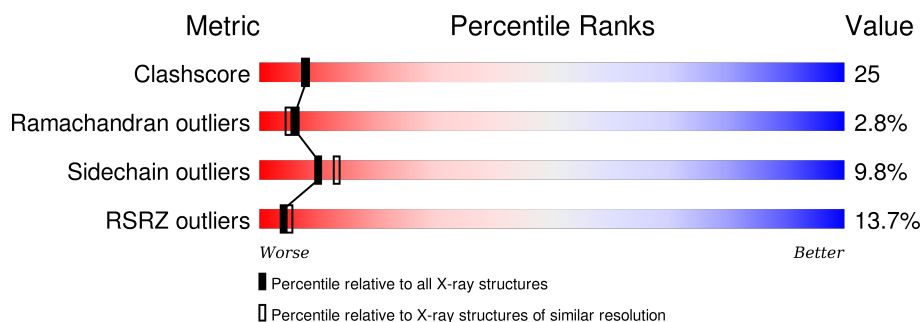
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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	102246	4595 (2.40-2.36)
Ramachandran outliers	100387	4520 (2.40-2.36)
Sidechain outliers	100360	4522 (2.40-2.36)
RSRZ outliers	91569	4034 (2.40-2.36)

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 ≥ 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	585	
1	B	585	

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
2	HLT	A	4001	-	-	X	X
2	HLT	A	4003	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	HLT	B	4001	-	-	X	X
2	HLT	B	4002	-	-	-	X
2	HLT	B	4003	-	-	-	X

2 Entry composition [i](#)

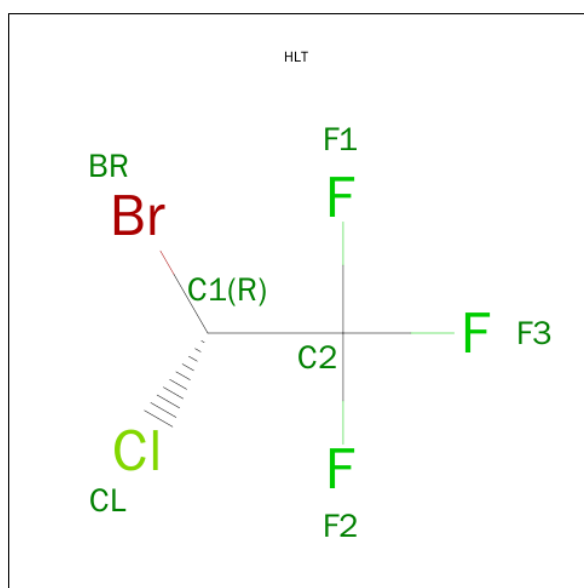
There are 3 unique types of molecules in this entry. The entry contains 8650 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SERUM ALBUMIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	578	Total	C	N	O	S	0	0	0
			4303	2732	728	803	40			
1	B	576	Total	C	N	O	S	0	0	0
			4248	2684	717	806	41			

- Molecule 2 is 2-BROMO-2-CHLORO-1,1,1-TRIFLUOROETHANE (three-letter code: HLT) (formula: $C_2HBrClF_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	Br	C	Cl	F	0	0
			7	1	2	1	3		
2	A	1	Total	Br	C	Cl	F	0	0
			7	1	2	1	3		
2	A	1	Total	Br	C	Cl	F	0	0
			7	1	2	1	3		
2	B	1	Total	Br	C	Cl	F	0	0
			7	1	2	1	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	Br	C	Cl	F	0	0
			7	1	2	1	3		
2	B	1	Total	Br	C	Cl	F	0	0
			7	1	2	1	3		

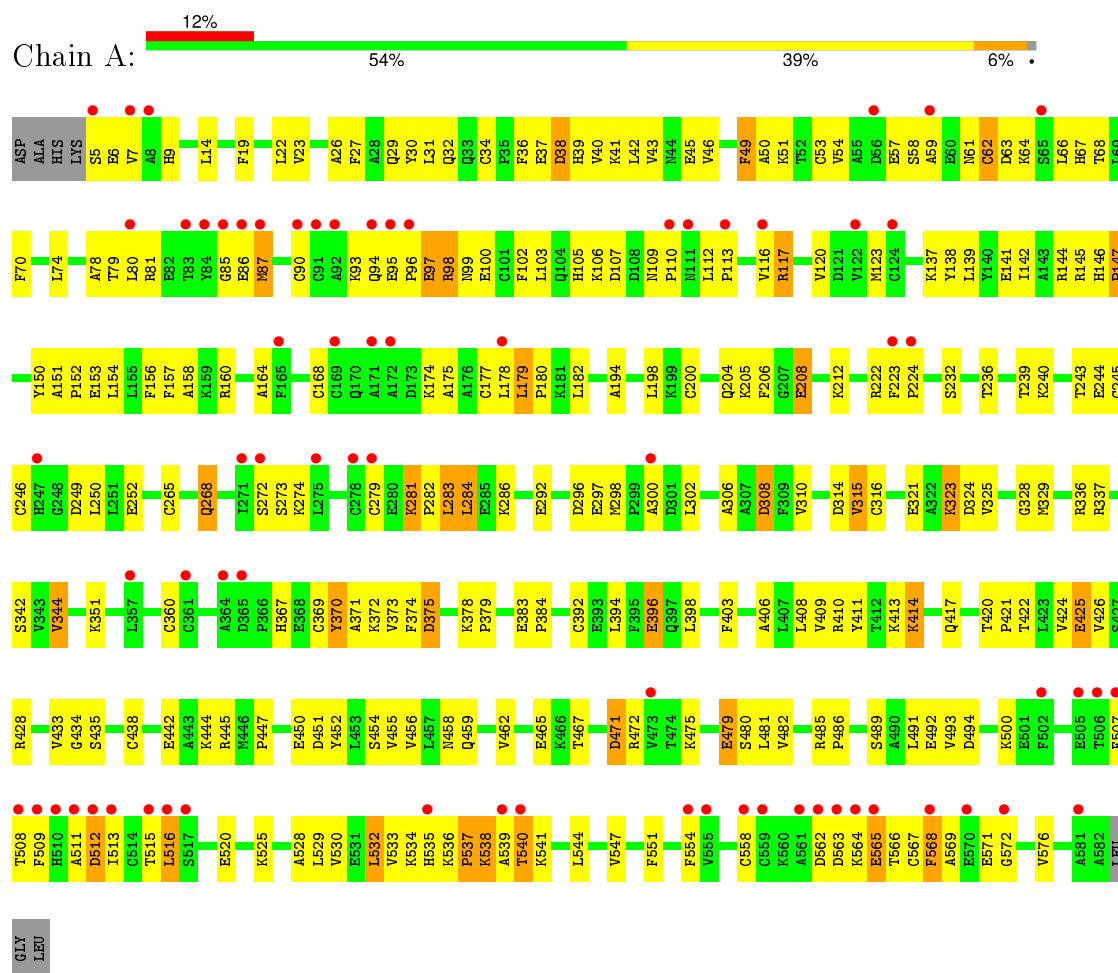
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	30	Total	O	0	0
			30	30		
3	B	27	Total	O	0	0
			27	27		

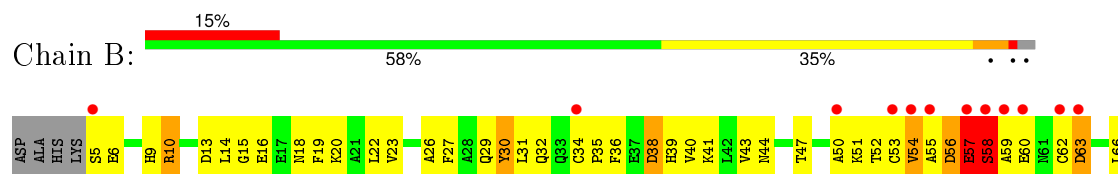
3 Residue-property plots [i](#)

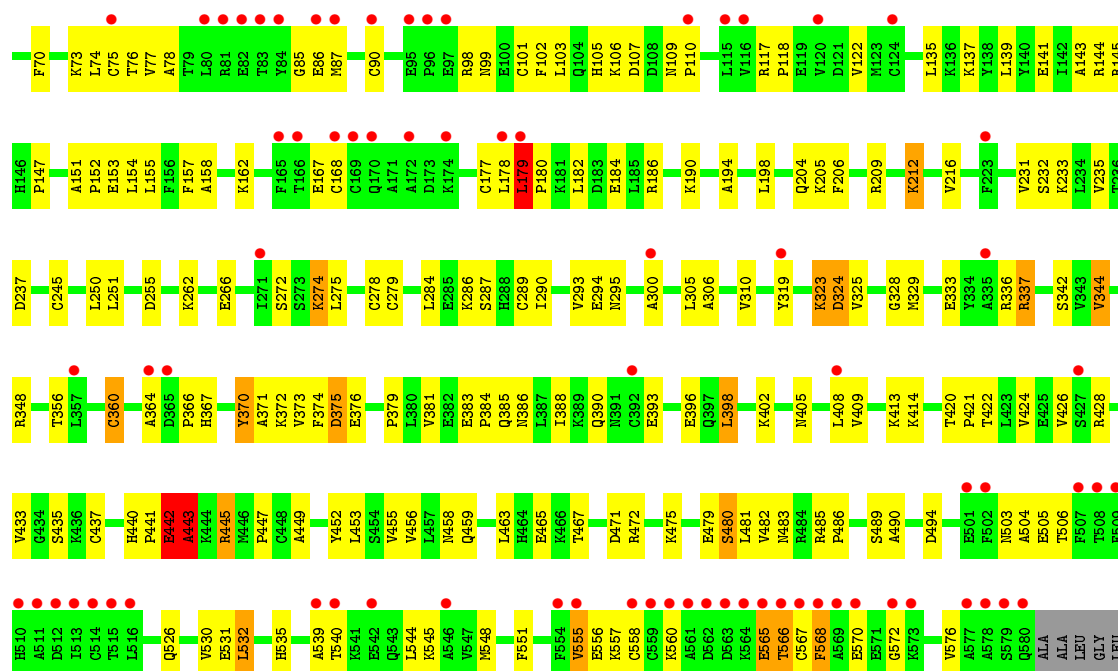
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: SERUM ALBUMIN



• Molecule 1: SERUM ALBUMIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	54.58 Å 54.96 Å 120.00 Å 81.39° 90.79° 65.55°	Depositor
Resolution (Å)	17.00 – 2.38 14.97 – 2.38	Depositor EDS
% Data completeness (in resolution range)	96.0 (17.00-2.38) 91.1 (14.97-2.38)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 2.37 Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.270 , 0.303 0.266 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	53.4	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 80.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 47994 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8650	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.50% 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, 0.375 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: HLT

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	0.34	0/4388	0.58	1/5965 (0.0%)
1	B	0.34	1/4329 (0.0%)	0.54	2/5892 (0.0%)
All	All	0.34	1/8717 (0.0%)	0.56	3/11857 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	442	GLU	CB-CG	7.29	1.66	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	443	ALA	N-CA-C	-6.56	93.28	111.00
1	B	539	ALA	N-CA-C	5.88	126.89	111.00
1	A	541	LYS	N-CA-C	-5.30	96.68	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	4303	0	3992	233	0
1	B	4248	0	3880	175	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	21	0	0	2	0
2	B	21	0	0	4	0
3	A	30	0	0	2	0
3	B	27	0	0	1	0
All	All	8650	0	7872	409	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 (409) 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:A:67:HIS:HB3	1:A:98:ARG:HH21	1.27	0.99
1:A:540:THR:HG23	1:A:544:LEU:HG	1.42	0.98
1:A:98:ARG:HH11	1:A:98:ARG:H	1.05	0.95
1:B:556:GLU:HG3	1:B:557:LYS:H	1.38	0.89
1:A:383:GLU:HB3	1:A:384:PRO:HD3	1.55	0.88
1:A:53:CYS:O	1:A:57:GLU:HG2	1.74	0.87
1:A:328:GLY:HA2	2:A:4001:HLT:BR	2.30	0.87
1:B:151:ALA:HB3	1:B:152:PRO:HD3	1.57	0.87
1:B:106:LYS:HD3	1:B:147:PRO:HB2	1.55	0.86
1:A:511:ALA:HB2	1:A:565:GLU:HB3	1.56	0.86
1:A:485:ARG:HB3	1:A:486:PRO:HD3	1.57	0.85
1:B:409:VAL:HG12	1:B:413:LYS:HE3	1.59	0.84
1:A:367:HIS:O	1:A:371:ALA:HB2	1.78	0.83
1:B:441:PRO:O	1:B:443:ALA:N	2.11	0.83
1:A:98:ARG:NH1	1:A:99:ASN:H	1.76	0.83
1:B:383:GLU:HB3	1:B:384:PRO:HD3	1.59	0.82
1:A:281:LYS:HB2	1:A:282:PRO:HD2	1.62	0.81
1:B:39:HIS:O	1:B:43:VAL:HG23	1.80	0.81
1:A:297:GLU:O	1:A:297:GLU:CA	2.29	0.81
1:A:472:ARG:HH12	1:A:494:ASP:HA	1.47	0.79
1:A:94:GLN:O	1:A:98:ARG:HB3	1.84	0.78
1:A:424:VAL:O	1:A:428:ARG:HG3	1.81	0.78
1:A:98:ARG:CZ	1:A:99:ASN:HB2	2.15	0.77
1:A:151:ALA:HB3	1:A:152:PRO:HD3	1.67	0.76
1:A:511:ALA:HA	1:A:568:PHE:CE2	2.20	0.75
1:A:14:LEU:HD13	1:A:22:LEU:HD12	1.68	0.75
1:A:306:ALA:HA	1:A:310:VAL:HG22	1.69	0.75
1:A:378:LYS:HB3	1:A:379:PRO:HD3	1.67	0.75
1:A:425:GLU:OE1	1:A:425:GLU:HA	1.85	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:LEU:HD21	1:B:155:LEU:HD11	1.68	0.75
1:B:556:GLU:HG3	1:B:557:LYS:N	2.01	0.75
1:A:558:CYS:HA	1:A:567:CYS:SG	2.27	0.74
1:A:198:LEU:HA	1:A:458:ASN:ND2	2.02	0.74
1:A:98:ARG:HH11	1:A:98:ARG:N	1.85	0.73
1:B:433:VAL:HG22	1:B:452:TYR:CD2	2.24	0.73
1:B:531:GLU:O	1:B:535:HIS:HD2	1.72	0.72
1:A:98:ARG:NH2	1:A:99:ASN:HB2	2.03	0.72
1:A:323:LYS:HG3	1:A:324:ASP:N	2.04	0.72
1:A:110:PRO:HG2	1:A:145:ARG:HA	1.72	0.71
1:A:26:ALA:HB2	1:A:250:LEU:HD12	1.70	0.71
1:A:564:LYS:O	1:A:566:THR:N	2.19	0.71
1:B:373:VAL:HG13	1:B:374:PHE:HD1	1.56	0.71
1:A:511:ALA:HB2	1:A:565:GLU:CB	2.20	0.71
1:A:540:THR:CG2	1:A:544:LEU:HG	2.20	0.70
1:A:120:VAL:HG21	1:A:175:ALA:HA	1.73	0.70
1:B:262:LYS:O	1:B:266:GLU:HG3	1.92	0.70
1:A:516:LEU:HD22	1:A:520:GLU:OE1	1.91	0.70
1:B:279:CYS:HA	1:B:286:LYS:HD2	1.74	0.70
1:A:141:GLU:OE1	1:A:144:ARG:HD3	1.92	0.69
1:B:16:GLU:O	1:B:20:LYS:HG2	1.92	0.69
1:A:34:CYS:HB3	1:A:39:HIS:NE2	2.08	0.69
1:B:52:THR:HA	1:B:56:ASP:OD2	1.92	0.69
1:A:179:LEU:HB2	1:A:180:PRO:HD3	1.75	0.69
1:A:279:CYS:HA	1:A:286:LYS:HD2	1.74	0.69
1:B:306:ALA:HA	1:B:310:VAL:HG22	1.75	0.68
1:B:34:CYS:HB3	1:B:39:HIS:NE2	2.09	0.68
1:A:98:ARG:NH1	1:A:98:ARG:H	1.87	0.68
1:A:110:PRO:C	1:A:112:LEU:H	1.96	0.68
1:A:107:ASP:O	1:A:147:PRO:HG2	1.94	0.67
1:B:449:ALA:O	1:B:453:LEU:HG	1.95	0.66
1:A:87:MET:HE3	1:A:105:HIS:HB3	1.76	0.66
1:A:141:GLU:O	1:A:145:ARG:HG3	1.95	0.65
1:A:208:GLU:OE2	1:A:212:LYS:HE3	1.96	0.65
1:B:367:HIS:O	1:B:371:ALA:HB2	1.96	0.65
1:B:420:THR:HB	1:B:421:PRO:HD3	1.78	0.65
1:B:373:VAL:HG13	1:B:374:PHE:CD1	2.31	0.65
1:B:153:GLU:O	1:B:157:PHE:HD1	1.80	0.65
1:A:23:VAL:O	1:A:27:PHE:HD1	1.78	0.65
1:B:424:VAL:O	1:B:428:ARG:HG3	1.97	0.64
1:B:26:ALA:HB2	1:B:250:LEU:HD12	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:ARG:NH1	1:A:494:ASP:HA	2.13	0.64
1:A:106:LYS:HD3	1:A:147:PRO:HB3	1.78	0.64
1:B:310:VAL:HG11	1:B:374:PHE:CE1	2.32	0.64
1:A:471:ASP:N	1:A:471:ASP:OD1	2.26	0.64
1:B:15:GLY:O	1:B:19:PHE:HB3	1.98	0.64
1:A:511:ALA:CB	1:A:565:GLU:HB3	2.28	0.63
1:A:7:VAL:HG22	1:A:66:LEU:HD23	1.81	0.63
1:A:394:LEU:HD11	1:A:398:LEU:HD11	1.80	0.63
1:A:67:HIS:CB	1:A:98:ARG:HH21	2.08	0.63
1:A:138:TYR:CE1	1:A:142:ILE:HD11	2.34	0.63
1:B:23:VAL:O	1:B:27:PHE:HD1	1.82	0.62
1:A:507:PHE:HD1	1:A:509:PHE:CE2	2.17	0.62
1:A:383:GLU:HB3	1:A:384:PRO:CD	2.29	0.62
1:A:281:LYS:HB2	1:A:282:PRO:CD	2.29	0.62
1:A:283:LEU:HG	1:A:284:LEU:HD23	1.81	0.62
1:B:141:GLU:O	1:B:145:ARG:HG3	1.98	0.62
1:A:420:THR:HB	1:A:421:PRO:HD3	1.82	0.62
1:A:406:ALA:O	1:A:409:VAL:HG12	2.00	0.61
1:B:22:LEU:CD2	1:B:155:LEU:HD11	2.29	0.61
1:A:472:ARG:HH21	1:A:491:LEU:HD22	1.65	0.61
1:A:297:GLU:CA	1:A:298:MET:N	2.63	0.61
1:A:205:LYS:HE3	1:A:465:GLU:OE2	2.00	0.61
1:B:90:CYS:O	1:B:98:ARG:HG3	2.01	0.60
1:A:433:VAL:HG22	1:A:452:TYR:CD2	2.36	0.60
1:B:290:ILE:O	1:B:293:VAL:HG12	2.01	0.60
1:A:507:PHE:HZ	1:A:576:VAL:HG22	1.67	0.60
1:A:39:HIS:O	1:A:43:VAL:HG23	2.02	0.60
1:A:31:LEU:HG	1:A:74:LEU:HD22	1.82	0.60
1:B:233:LYS:HE3	1:B:237:ASP:OD2	2.01	0.59
1:A:572:GLY:O	1:A:576:VAL:HG23	2.02	0.59
1:B:14:LEU:HD13	1:B:22:LEU:HD12	1.84	0.59
1:B:556:GLU:O	1:B:560:LYS:HG2	2.02	0.59
1:B:59:ALA:HB3	1:B:62:CYS:SG	2.43	0.59
1:A:49:PHE:HE1	1:A:62:CYS:SG	2.25	0.59
1:A:281:LYS:CB	1:A:282:PRO:HD2	2.33	0.59
1:A:141:GLU:OE1	1:A:141:GLU:HA	2.03	0.59
1:B:485:ARG:HB3	1:B:486:PRO:HD3	1.84	0.58
1:B:437:CYS:O	1:B:440:HIS:HB2	2.02	0.58
1:A:34:CYS:HB3	1:A:39:HIS:HE2	1.67	0.58
1:A:61:ASN:O	1:A:64:LYS:HB2	2.03	0.58
1:B:323:LYS:HG3	1:B:324:ASP:N	2.19	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:GLN:HG2	1:B:143:ALA:O	2.03	0.58
1:A:328:GLY:CA	2:A:4001:HLT:BR	3.06	0.58
1:A:66:LEU:O	1:A:70:PHE:HD2	1.84	0.58
1:B:212:LYS:O	1:B:216:VAL:HG23	2.03	0.57
1:A:485:ARG:HB3	1:A:486:PRO:CD	2.31	0.57
1:B:475:LYS:O	1:B:479:GLU:HB2	2.03	0.57
1:B:5:SER:HA	1:B:62:CYS:O	2.05	0.57
1:A:297:GLU:O	1:A:298:MET:N	2.38	0.57
1:A:49:PHE:CE1	1:A:53:CYS:SG	2.98	0.56
1:A:507:PHE:HD1	1:A:509:PHE:CD2	2.22	0.56
1:B:325:VAL:HG12	1:B:329:MET:CE	2.35	0.56
1:A:206:PHE:CE2	1:A:481:LEU:HD13	2.40	0.56
1:B:433:VAL:HG22	1:B:452:TYR:HD2	1.71	0.56
1:A:178:LEU:O	1:A:179:LEU:C	2.43	0.56
1:A:511:ALA:HA	1:A:568:PHE:CD2	2.40	0.56
1:A:138:TYR:CZ	1:A:142:ILE:HD11	2.41	0.56
1:A:99:ASN:HA	1:A:102:PHE:HD2	1.71	0.55
1:A:38:ASP:OD1	1:A:38:ASP:N	2.38	0.55
1:A:297:GLU:O	1:A:298:MET:HA	2.06	0.55
1:A:156:PHE:CE1	1:A:160:ARG:HD2	2.42	0.55
1:A:87:MET:CE	1:A:105:HIS:HB3	2.37	0.54
1:B:408:LEU:HD11	1:B:526:GLN:HB3	1.89	0.54
1:B:405:ASN:O	1:B:409:VAL:HG23	2.07	0.54
1:B:306:ALA:CA	1:B:310:VAL:HG22	2.37	0.54
1:A:38:ASP:O	1:A:42:LEU:HG	2.08	0.54
1:A:408:LEU:HD23	1:A:529:LEU:HD23	1.88	0.54
1:B:198:LEU:HA	1:B:458:ASN:ND2	2.22	0.54
1:A:49:PHE:HE1	1:A:53:CYS:SG	2.31	0.54
1:A:511:ALA:CB	1:A:565:GLU:CB	2.85	0.54
1:A:567:CYS:O	1:A:571:GLU:N	2.36	0.54
1:A:145:ARG:O	1:A:146:HIS:HD2	1.89	0.54
1:A:408:LEU:HD21	1:A:530:VAL:HG23	1.90	0.54
1:A:249:ASP:HB3	1:A:252:GLU:CD	2.28	0.54
1:B:383:GLU:HB3	1:B:384:PRO:CD	2.35	0.54
1:A:564:LYS:C	1:A:566:THR:H	2.09	0.54
1:A:32:GLN:NE2	1:A:147:PRO:HG3	2.23	0.54
1:B:98:ARG:O	1:B:101:CYS:HB3	2.08	0.54
1:A:452:TYR:O	1:A:456:VAL:HG23	2.07	0.54
1:B:274:LYS:CE	1:B:294:GLU:HG3	2.38	0.54
1:A:178:LEU:HG	1:A:182:LEU:HG	1.88	0.53
1:B:186:ARG:O	1:B:190:LYS:HG3	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:LYS:CB	1:A:282:PRO:CD	2.85	0.53
1:B:54:VAL:HG12	1:B:55:ALA:N	2.23	0.53
1:A:533:VAL:HG12	1:A:533:VAL:O	2.09	0.53
1:A:139:LEU:HD21	1:A:158:ALA:HB2	1.91	0.53
1:A:283:LEU:HG	1:A:284:LEU:N	2.22	0.53
1:A:49:PHE:O	1:A:49:PHE:HD1	1.91	0.53
1:B:370:TYR:C	1:B:370:TYR:CD1	2.81	0.53
1:A:372:LYS:O	1:A:375:ASP:HB2	2.09	0.53
1:A:558:CYS:CB	1:A:567:CYS:SG	2.97	0.53
1:A:370:TYR:CD1	1:A:370:TYR:C	2.83	0.52
1:A:23:VAL:HG13	1:A:70:PHE:HE1	1.73	0.52
1:B:565:GLU:HG3	1:B:565:GLU:O	2.08	0.52
1:B:348:ARG:HG3	1:B:482:VAL:HG12	1.90	0.52
1:A:351:LYS:HD3	3:A:2016:HOH:O	2.08	0.52
1:A:94:GLN:O	1:A:98:ARG:HD3	2.09	0.52
1:A:562:ASP:OD1	1:A:562:ASP:O	2.26	0.52
1:A:99:ASN:HA	1:A:102:PHE:CD2	2.45	0.52
1:A:530:VAL:O	1:A:534:LYS:HG3	2.09	0.52
1:B:99:ASN:HA	1:B:102:PHE:HD2	1.74	0.52
1:B:422:THR:O	1:B:426:VAL:HG23	2.09	0.52
1:A:30:TYR:HE1	1:A:103:LEU:HD23	1.75	0.52
1:A:5:SER:HA	1:A:62:CYS:O	2.10	0.52
1:A:507:PHE:CD1	1:A:509:PHE:CE2	2.98	0.52
1:A:41:LYS:O	1:A:45:GLU:HG3	2.09	0.52
1:B:205:LYS:HE2	1:B:465:GLU:OE1	2.10	0.52
1:A:509:PHE:CZ	1:A:551:PHE:CZ	2.98	0.51
1:B:14:LEU:HD13	1:B:22:LEU:CD1	2.39	0.51
1:A:116:VAL:HG22	1:A:117:ARG:N	2.24	0.51
1:B:342:SER:OG	1:B:344:VAL:HG23	2.10	0.51
1:B:36:PHE:O	1:B:40:VAL:HG23	2.10	0.51
1:A:558:CYS:CA	1:A:567:CYS:SG	2.97	0.51
1:B:558:CYS:SG	1:B:568:PHE:N	2.83	0.51
1:B:356:THR:O	1:B:360:CYS:HB2	2.11	0.51
1:A:239:THR:O	1:A:243:THR:OG1	2.27	0.51
1:B:422:THR:HG23	1:B:463:LEU:HD13	1.93	0.51
1:B:551:PHE:O	1:B:555:VAL:HG23	2.10	0.51
1:B:504:ALA:C	1:B:506:THR:H	2.13	0.51
1:A:279:CYS:HA	1:A:286:LYS:CD	2.38	0.51
1:A:373:VAL:HG13	1:A:374:PHE:CD1	2.46	0.51
1:A:342:SER:HA	1:A:447:PRO:HA	1.93	0.51
1:B:10:ARG:NH1	1:B:255:ASP:OD2	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:PHE:CD1	1:B:19:PHE:C	2.84	0.51
1:B:23:VAL:O	1:B:27:PHE:CD1	2.64	0.51
1:A:106:LYS:HD3	1:A:147:PRO:CB	2.41	0.51
1:B:480:SER:OG	1:B:483:ASN:HB2	2.11	0.51
1:A:66:LEU:HB3	1:A:70:PHE:CE2	2.45	0.50
1:B:107:ASP:HB3	1:B:110:PRO:HG3	1.92	0.50
1:B:398:LEU:O	1:B:402:LYS:HB2	2.11	0.50
1:B:118:PRO:HB2	1:B:122:VAL:HB	1.92	0.50
1:A:344:VAL:HG12	1:A:482:VAL:HG13	1.93	0.50
1:A:6:GLU:O	1:A:9:HIS:HB3	2.10	0.50
1:B:384:PRO:O	1:B:388:ILE:HG12	2.11	0.50
1:B:57:GLU:OE1	1:B:57:GLU:HA	2.10	0.50
1:A:67:HIS:CE1	1:A:99:ASN:ND2	2.80	0.50
1:A:297:GLU:O	1:A:298:MET:CA	2.60	0.50
1:B:566:THR:O	1:B:570:GLU:N	2.45	0.49
1:A:49:PHE:CD1	1:A:49:PHE:C	2.85	0.49
1:B:274:LYS:HE3	1:B:294:GLU:HG3	1.93	0.49
1:B:490:ALA:HB3	3:B:2024:HOH:O	2.10	0.49
1:B:370:TYR:C	1:B:370:TYR:HD1	2.15	0.49
1:A:51:LYS:HA	1:A:54:VAL:HG23	1.95	0.49
1:A:392:CYS:O	1:A:396:GLU:HG3	2.12	0.49
1:A:422:THR:O	1:A:426:VAL:HG23	2.13	0.49
1:A:564:LYS:C	1:A:566:THR:N	2.65	0.49
1:A:36:PHE:O	1:A:40:VAL:HG23	2.13	0.49
1:B:30:TYR:HE1	1:B:103:LEU:HD23	1.78	0.49
1:B:209:ARG:HG2	2:B:4001:HLT:F2	2.03	0.49
1:B:328:GLY:HA2	2:B:4001:HLT:BR	2.69	0.48
1:B:558:CYS:HB3	1:B:568:PHE:CD2	2.48	0.48
1:B:386:ASN:O	1:B:390:GLN:HB2	2.14	0.48
1:A:168:CYS:SG	1:A:177:CYS:C	2.91	0.48
1:A:179:LEU:HB2	1:A:180:PRO:CD	2.43	0.48
1:A:49:PHE:HD1	1:A:49:PHE:C	2.17	0.48
1:A:507:PHE:HZ	1:A:576:VAL:CG2	2.26	0.48
1:B:545:LYS:HA	1:B:548:MET:HB2	1.95	0.48
1:A:50:ALA:O	1:A:54:VAL:HG23	2.13	0.48
1:B:194:ALA:HB1	1:B:455:VAL:CG1	2.43	0.48
1:B:279:CYS:HA	1:B:286:LYS:CD	2.43	0.48
1:B:32:GLN:NE2	1:B:110:PRO:HG3	2.28	0.48
1:A:81:ARG:CB	1:A:85:GLY:HA2	2.44	0.48
1:A:200:CYS:O	1:A:204:GLN:HG3	2.13	0.48
1:A:314:ASP:O	1:A:315:VAL:C	2.52	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:VAL:HG13	1:A:374:PHE:HD1	1.78	0.48
1:A:509:PHE:CZ	1:A:551:PHE:CE1	3.01	0.48
1:A:475:LYS:O	1:A:479:GLU:HB2	2.13	0.48
1:B:106:LYS:HD3	1:B:147:PRO:CB	2.37	0.48
1:B:319:TYR:CE1	1:B:323:LYS:HB2	2.49	0.47
1:A:325:VAL:HG12	1:A:329:MET:HE2	1.94	0.47
1:A:29:GLN:HG2	1:A:147:PRO:HA	1.95	0.47
1:B:503:ASN:OD1	1:B:504:ALA:N	2.47	0.47
1:A:51:LYS:HA	1:A:54:VAL:CG2	2.45	0.47
1:A:110:PRO:C	1:A:112:LEU:N	2.64	0.47
1:A:41:LYS:HE3	1:A:42:LEU:HD23	1.97	0.47
1:B:107:ASP:O	1:B:110:PRO:HD3	2.14	0.47
1:A:98:ARG:NH1	1:A:99:ASN:HB2	2.30	0.47
1:A:511:ALA:O	1:A:513:ILE:N	2.48	0.47
1:B:135:LEU:HD11	1:B:162:LYS:HB2	1.96	0.47
1:B:50:ALA:O	1:B:54:VAL:HG23	2.14	0.47
1:B:409:VAL:CG1	1:B:413:LYS:HE3	2.39	0.47
1:A:41:LYS:HE3	1:A:42:LEU:CD2	2.45	0.47
1:B:558:CYS:SG	1:B:567:CYS:C	2.94	0.47
1:A:563:ASP:C	1:A:564:LYS:O	2.49	0.47
1:A:42:LEU:O	1:A:46:VAL:HG23	2.15	0.47
1:B:32:GLN:NE2	1:B:110:PRO:CG	2.78	0.47
1:B:178:LEU:HG	1:B:182:LEU:HG	1.96	0.47
1:A:425:GLU:OE1	1:A:425:GLU:CA	2.60	0.46
1:B:364:ALA:O	1:B:366:PRO:HD3	2.14	0.46
1:B:206:PHE:CE2	1:B:481:LEU:HD13	2.51	0.46
1:B:572:GLY:O	1:B:576:VAL:HG23	2.15	0.46
1:A:223:PHE:CD1	1:A:272:SER:HB2	2.50	0.46
1:B:388:ILE:HG21	1:B:445:ARG:HB3	1.96	0.46
1:A:153:GLU:O	1:A:157:PHE:HD2	1.97	0.46
1:B:531:GLU:O	1:B:535:HIS:CD2	2.61	0.46
1:B:472:ARG:HH12	1:B:494:ASP:CA	2.27	0.46
1:A:66:LEU:HB3	1:A:70:PHE:HE2	1.80	0.46
1:A:403:PHE:O	1:A:406:ALA:HB3	2.16	0.46
1:B:504:ALA:C	1:B:506:THR:N	2.69	0.46
1:B:376:GLU:O	1:B:379:PRO:HD2	2.15	0.46
1:B:63:ASP:OD1	1:B:63:ASP:O	2.34	0.46
1:B:472:ARG:NH1	1:B:494:ASP:CB	2.79	0.46
1:B:31:LEU:HG	1:B:74:LEU:HD22	1.98	0.46
1:B:73:LYS:O	1:B:76:THR:HG23	2.16	0.46
1:A:507:PHE:CZ	1:A:576:VAL:HG22	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:LYS:O	1:B:141:GLU:HG2	2.16	0.46
1:B:44:ASN:HA	1:B:47:THR:HG22	1.98	0.46
1:A:459:GLN:O	1:A:462:VAL:HG22	2.16	0.46
1:B:441:PRO:O	1:B:442:GLU:C	2.52	0.46
1:A:373:VAL:HG13	1:A:374:PHE:N	2.31	0.46
1:A:532:LEU:HD11	1:A:547:VAL:HG11	1.98	0.46
1:A:310:VAL:O	1:A:370:TYR:HE1	1.98	0.45
1:A:61:ASN:C	1:A:63:ASP:N	2.69	0.45
1:A:360:CYS:SG	1:A:370:TYR:N	2.90	0.45
1:A:409:VAL:HG13	1:A:410:ARG:N	2.31	0.45
1:B:57:GLU:O	1:B:59:ALA:N	2.50	0.45
1:B:51:LYS:C	1:B:53:CYS:H	2.20	0.45
1:B:372:LYS:O	1:B:375:ASP:HB2	2.17	0.45
1:B:381:VAL:O	1:B:385:GLN:HG3	2.15	0.45
1:A:90:CYS:HA	1:A:93:LYS:HG3	1.98	0.45
1:B:393:GLU:HA	1:B:396:GLU:HG3	1.98	0.45
1:B:342:SER:HA	1:B:447:PRO:HA	1.99	0.45
1:B:472:ARG:NH1	1:B:494:ASP:HA	2.32	0.45
1:A:554:PHE:CZ	1:A:568:PHE:HD1	2.35	0.45
1:A:81:ARG:CA	1:A:85:GLY:HA2	2.47	0.45
1:A:98:ARG:HG2	1:A:99:ASN:N	2.30	0.45
1:A:509:PHE:CE1	1:A:551:PHE:CZ	3.04	0.45
1:A:554:PHE:CE1	1:A:572:GLY:HA2	2.52	0.45
1:A:120:VAL:HG21	1:A:175:ALA:CA	2.44	0.45
1:B:141:GLU:OE1	1:B:144:ARG:HD3	2.16	0.45
1:A:351:LYS:CD	3:A:2016:HOH:O	2.62	0.45
1:B:472:ARG:NH1	1:B:494:ASP:CA	2.80	0.45
1:A:413:LYS:NZ	1:A:537:PRO:O	2.50	0.45
1:A:117:ARG:HG3	1:A:123:MET:HE3	1.97	0.44
1:A:492:GLU:HG3	1:A:493:VAL:H	1.81	0.44
1:A:67:HIS:CE1	1:A:99:ASN:HD21	2.35	0.44
1:A:538:LYS:O	1:A:539:ALA:C	2.55	0.44
1:B:456:VAL:O	1:B:459:GLN:HB3	2.17	0.44
1:A:434:GLY:O	1:A:438:CYS:HB2	2.17	0.44
1:B:139:LEU:HD22	1:B:154:LEU:HG	2.00	0.44
1:B:87:MET:HE3	1:B:105:HIS:HB3	1.99	0.44
1:A:507:PHE:CD1	1:A:509:PHE:HE2	2.34	0.44
1:B:139:LEU:HD21	1:B:158:ALA:HB2	1.99	0.44
1:A:566:THR:O	1:A:569:ALA:N	2.48	0.44
1:A:61:ASN:O	1:A:63:ASP:N	2.50	0.44
1:B:70:PHE:CD1	1:B:70:PHE:N	2.86	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:LYS:O	1:A:528:ALA:HB3	2.17	0.44
1:A:265:CYS:SG	1:A:286:LYS:HD2	2.58	0.44
1:A:420:THR:HG23	1:A:530:VAL:CG1	2.47	0.44
1:A:325:VAL:HG12	1:A:329:MET:CE	2.47	0.44
1:A:179:LEU:O	1:A:180:PRO:C	2.56	0.44
1:A:14:LEU:HD13	1:A:22:LEU:CD1	2.42	0.44
1:B:141:GLU:HA	1:B:141:GLU:OE1	2.18	0.44
1:A:204:GLN:HE21	1:A:246:CYS:HB3	1.82	0.44
1:A:19:PHE:C	1:A:19:PHE:CD1	2.91	0.44
1:A:500:LYS:O	1:A:535:HIS:CD2	2.71	0.43
1:B:135:LEU:HD11	1:B:162:LYS:HD3	2.00	0.43
1:B:540:THR:CB	1:B:544:LEU:HG	2.47	0.43
1:B:30:TYR:CE1	1:B:103:LEU:HD23	2.53	0.43
1:B:373:VAL:C	1:B:375:ASP:H	2.21	0.43
1:B:9:HIS:O	1:B:13:ASP:HB2	2.18	0.43
1:A:512:ASP:O	1:A:515:THR:HG22	2.19	0.43
1:A:394:LEU:CD1	1:A:398:LEU:HD11	2.47	0.43
1:B:6:GLU:HG2	1:B:66:LEU:HD11	2.01	0.43
1:A:360:CYS:SG	1:A:369:CYS:C	2.97	0.43
1:A:274:LYS:HE3	1:A:296:ASP:HA	2.01	0.43
1:A:95:GLU:O	1:A:96:PRO:C	2.57	0.43
1:A:451:ASP:O	1:A:454:SER:HB2	2.18	0.43
1:B:422:THR:HG23	1:B:463:LEU:CD1	2.49	0.43
1:B:209:ARG:CG	2:B:4001:HLT:F2	2.56	0.43
1:A:509:PHE:CE1	1:A:551:PHE:HZ	2.36	0.43
1:B:272:SER:HB3	1:B:275:LEU:HG	2.01	0.43
1:B:310:VAL:CG1	1:B:374:PHE:CE1	3.01	0.43
1:B:367:HIS:HA	1:B:370:TYR:CZ	2.54	0.43
1:A:78:ALA:C	1:A:80:LEU:H	2.21	0.43
1:B:66:LEU:HD22	1:B:251:LEU:HD12	2.00	0.42
1:A:95:GLU:O	1:A:97:GLU:N	2.52	0.42
1:B:442:GLU:HA	1:B:445:ARG:HD2	2.00	0.42
1:B:56:ASP:N	1:B:56:ASP:OD1	2.52	0.42
1:B:98:ARG:HG2	1:B:102:PHE:CE2	2.54	0.42
1:B:117:ARG:HA	1:B:118:PRO:HD3	1.85	0.42
1:A:536:LYS:N	1:A:537:PRO:HD3	2.33	0.42
1:B:75:CYS:HA	1:B:78:ALA:HB3	2.01	0.42
1:A:240:LYS:HE2	1:A:244:GLU:OE2	2.19	0.42
1:A:194:ALA:HB1	1:A:455:VAL:CG1	2.50	0.42
1:B:374:PHE:CD1	1:B:374:PHE:N	2.87	0.42
1:B:532:LEU:HA	1:B:532:LEU:HD23	1.88	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:531:GLU:HA	1:B:531:GLU:OE1	2.19	0.42
1:A:408:LEU:HD11	1:A:530:VAL:CG2	2.49	0.42
1:A:61:ASN:C	1:A:63:ASP:H	2.21	0.42
1:B:179:LEU:HB2	1:B:180:PRO:HD3	2.01	0.42
1:B:168:CYS:SG	1:B:177:CYS:C	2.98	0.42
1:A:100:GLU:HA	1:A:100:GLU:OE1	2.20	0.42
1:B:30:TYR:OH	1:B:103:LEU:HD21	2.20	0.42
1:A:420:THR:HG23	1:A:530:VAL:HG11	2.02	0.42
1:B:57:GLU:HB3	1:B:58:SER:H	1.52	0.42
1:B:485:ARG:O	1:B:486:PRO:C	2.58	0.42
1:B:30:TYR:HA	1:B:30:TYR:HD1	1.74	0.42
1:B:70:PHE:N	1:B:70:PHE:HD1	2.17	0.42
1:A:222:ARG:C	1:A:224:PRO:HD3	2.40	0.42
1:A:99:ASN:O	1:A:103:LEU:HG	2.19	0.42
1:B:178:LEU:O	1:B:179:LEU:C	2.58	0.42
1:A:492:GLU:O	1:A:493:VAL:C	2.57	0.42
1:A:539:ALA:O	1:A:540:THR:OG1	2.33	0.42
1:B:151:ALA:HB3	1:B:152:PRO:CD	2.39	0.42
1:B:373:VAL:C	1:B:375:ASP:N	2.73	0.42
1:A:535:HIS:O	1:A:535:HIS:ND1	2.52	0.42
1:A:417:GLN:H	1:A:417:GLN:CD	2.23	0.42
1:B:34:CYS:HA	1:B:35:PRO:HD3	1.90	0.41
1:B:374:PHE:N	1:B:374:PHE:HD1	2.18	0.41
1:B:408:LEU:HD23	1:B:408:LEU:HA	1.94	0.41
1:B:278:CYS:HB3	1:B:289:CYS:HB3	1.91	0.41
1:A:370:TYR:HD1	1:A:370:TYR:C	2.22	0.41
1:A:110:PRO:HB3	1:A:112:LEU:HG	2.01	0.41
1:A:308:ASP:N	1:A:308:ASP:OD1	2.53	0.41
1:A:97:GLU:CB	1:A:100:GLU:CG	2.98	0.41
1:B:18:ASN:O	1:B:22:LEU:HG	2.21	0.41
1:B:109:ASN:O	1:B:110:PRO:C	2.58	0.41
1:B:29:GLN:HG3	1:B:143:ALA:HB1	2.01	0.41
1:A:302:LEU:HA	1:A:302:LEU:HD23	1.95	0.41
1:B:231:VAL:O	1:B:235:VAL:HG23	2.21	0.41
1:B:333:GLU:O	1:B:337:ARG:HG2	2.20	0.41
1:A:164:ALA:O	1:A:178:LEU:HD12	2.20	0.41
1:A:433:VAL:HG22	1:A:452:TYR:HD2	1.83	0.41
1:A:139:LEU:HD22	1:A:154:LEU:HG	2.03	0.41
1:A:394:LEU:O	1:A:398:LEU:HG	2.20	0.41
1:B:472:ARG:NH1	1:B:494:ASP:HB2	2.36	0.41
1:A:563:ASP:O	1:A:564:LYS:C	2.58	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:VAL:HG23	1:A:450:GLU:HG2	2.02	0.41
1:A:411:TYR:HA	1:A:414:LYS:HD3	2.01	0.41
1:B:408:LEU:HD22	1:B:530:VAL:CG2	2.51	0.41
1:B:32:GLN:HE21	1:B:110:PRO:HG2	1.86	0.41
2:B:4001:HLT:CL	2:B:4002:HLT:F1	2.66	0.41
1:A:315:VAL:HG12	1:A:316:CYS:N	2.35	0.41
1:B:38:ASP:O	1:B:41:LYS:HB3	2.21	0.41
1:A:378:LYS:HB3	1:A:379:PRO:CD	2.46	0.40
1:B:29:GLN:HG2	1:B:147:PRO:HA	2.02	0.40
1:A:507:PHE:CD1	1:A:509:PHE:CD2	3.07	0.40
1:B:179:LEU:HD22	1:B:179:LEU:HA	1.91	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	574/585 (98%)	498 (87%)	58 (10%)	18 (3%)	5 4
1	B	574/585 (98%)	493 (86%)	67 (12%)	14 (2%)	7 7
All	All	1148/1170 (98%)	991 (86%)	125 (11%)	32 (3%)	6 5

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	268	GLN
1	A	300	ALA
1	A	315	VAL
1	A	538	LYS
1	B	54	VAL
1	B	57	GLU
1	B	58	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	442	GLU
1	A	58	SER
1	A	59	ALA
1	A	512	ASP
1	A	540	THR
1	B	60	GLU
1	B	85	GLY
1	B	300	ALA
1	B	555	VAL
1	B	565	GLU
1	A	479	GLU
1	A	62	CYS
1	A	97	GLU
1	A	150	TYR
1	A	179	LEU
1	A	565	GLU
1	A	147	PRO
1	A	321	GLU
1	B	77	VAL
1	B	86	GLU
1	B	443	ALA
1	B	505	GLU
1	B	179	LEU
1	A	113	PRO
1	A	537	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	425/511 (83%)	381 (90%)	44 (10%)	9	11
1	B	415/511 (81%)	377 (91%)	38 (9%)	11	15
All	All	840/1022 (82%)	758 (90%)	82 (10%)	10	13

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	GLU
1	A	38	ASP
1	A	49	PHE
1	A	68	THR
1	A	79	THR
1	A	86	GLU
1	A	87	MET
1	A	98	ARG
1	A	109	ASN
1	A	117	ARG
1	A	137	LYS
1	A	174	LYS
1	A	208	GLU
1	A	232	SER
1	A	236	THR
1	A	245	CYS
1	A	268	GLN
1	A	273	SER
1	A	281	LYS
1	A	283	LEU
1	A	284	LEU
1	A	292	GLU
1	A	308	ASP
1	A	323	LYS
1	A	336	ARG
1	A	337	ARG
1	A	344	VAL
1	A	370	TYR
1	A	375	ASP
1	A	396	GLU
1	A	414	LYS
1	A	425	GLU
1	A	435	SER
1	A	442	GLU
1	A	444	LYS
1	A	445	ARG
1	A	467	THR
1	A	471	ASP
1	A	480	SER
1	A	489	SER
1	A	508	THR
1	A	516	LEU
1	A	532	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	568	PHE
1	B	10	ARG
1	B	30	TYR
1	B	38	ASP
1	B	56	ASP
1	B	57	GLU
1	B	58	SER
1	B	63	ASP
1	B	167	GLU
1	B	179	LEU
1	B	184	GLU
1	B	204	GLN
1	B	212	LYS
1	B	232	SER
1	B	245	CYS
1	B	274	LYS
1	B	284	LEU
1	B	287	SER
1	B	295	ASN
1	B	305	LEU
1	B	323	LYS
1	B	324	ASP
1	B	336	ARG
1	B	337	ARG
1	B	344	VAL
1	B	360	CYS
1	B	370	TYR
1	B	375	ASP
1	B	398	LEU
1	B	414	LYS
1	B	435	SER
1	B	445	ARG
1	B	467	THR
1	B	471	ASP
1	B	480	SER
1	B	489	SER
1	B	532	LEU
1	B	566	THR
1	B	568	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	HIS
1	A	109	ASN
1	A	146	HIS
1	A	204	GLN
1	A	318	ASN
1	A	385	GLN
1	A	458	ASN
1	A	483	ASN
1	B	32	GLN
1	B	196	GLN
1	B	386	ASN
1	B	483	ASN
1	B	535	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](#)

6 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	HLT	A	4001	-	4,6,6	0.36	0	3,9,9	1.26	0
2	HLT	A	4002	-	4,6,6	0.31	0	3,9,9	1.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HLT	A	4003	-	4,6,6	0.35	0	3,9,9	1.14	0
2	HLT	B	4001	-	4,6,6	0.46	0	3,9,9	1.23	0
2	HLT	B	4002	-	4,6,6	0.22	0	3,9,9	1.25	0
2	HLT	B	4003	-	4,6,6	0.29	0	3,9,9	1.28	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HLT	A	4001	-	-	0/3/6/6	0/0/0/0
2	HLT	A	4002	-	-	0/3/6/6	0/0/0/0
2	HLT	A	4003	-	-	0/3/6/6	0/0/0/0
2	HLT	B	4001	-	-	0/3/6/6	0/0/0/0
2	HLT	B	4002	-	-	0/3/6/6	0/0/0/0
2	HLT	B	4003	-	-	0/3/6/6	0/0/0/0

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.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4001	HLT	2	0
2	B	4001	HLT	4	0
2	B	4002	HLT	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	578/585 (98%)	0.68	72 (12%) 5 6	25, 69, 132, 144	0
1	B	576/585 (98%)	0.81	86 (14%) 3 4	34, 78, 137, 150	0
All	All	1154/1170 (98%)	0.74	158 (13%) 4 5	25, 73, 135, 150	0

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	539	ALA	12.0
1	B	539	ALA	10.9
1	B	563	ASP	10.5
1	B	562	ASP	7.8
1	A	96	PRO	7.6
1	B	83	THR	7.5
1	A	506	THR	6.0
1	B	577	ALA	5.8
1	A	568	PHE	5.8
1	B	508	THR	5.6
1	A	85	GLY	5.5
1	B	507	PHE	5.4
1	B	364	ALA	5.4
1	A	513	ILE	5.2
1	A	300	ALA	5.2
1	B	165	PHE	5.2
1	B	116	VAL	5.0
1	A	364	ALA	4.8
1	B	515	THR	4.8
1	A	505	GLU	4.8
1	B	558	CYS	4.7
1	B	172	ALA	4.5
1	B	567	CYS	4.4
1	B	540	THR	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	82	GLU	4.4
1	A	83	THR	4.4
1	A	116	VAL	4.3
1	A	563	ASP	4.3
1	A	516	LEU	4.1
1	A	565	GLU	4.1
1	B	569	ALA	4.1
1	B	578	ALA	4.1
1	B	502	PHE	4.0
1	B	512	ASP	4.0
1	A	56	ASP	3.9
1	B	546	ALA	3.8
1	A	271	ILE	3.8
1	A	84	TYR	3.8
1	B	516	LEU	3.8
1	A	507	PHE	3.7
1	B	365	ASP	3.7
1	A	357	LEU	3.7
1	B	509	PHE	3.7
1	A	510	HIS	3.6
1	B	511	ALA	3.6
1	B	60	GLU	3.6
1	A	581	ALA	3.5
1	A	178	LEU	3.5
1	B	566	THR	3.5
1	B	568	PHE	3.5
1	B	86	GLU	3.5
1	B	554	PHE	3.4
1	A	511	ALA	3.4
1	A	223	PHE	3.4
1	B	169	CYS	3.4
1	A	169	CYS	3.3
1	A	7	VAL	3.3
1	A	95	GLU	3.2
1	A	87	MET	3.2
1	A	91	CYS	3.2
1	B	96	PRO	3.2
1	B	55	ALA	3.2
1	B	570	GLU	3.1
1	B	513	ILE	3.1
1	A	275	LEU	3.0
1	A	122	VAL	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	223	PHE	2.9
1	A	90	CYS	2.9
1	A	558	CYS	2.9
1	B	124	CYS	2.9
1	B	97	GLU	2.9
1	A	561	ALA	2.9
1	A	172	ALA	2.9
1	B	58	SER	2.9
1	A	515	THR	2.9
1	B	62	CYS	2.9
1	A	508	THR	2.8
1	A	111	ASN	2.8
1	B	572	GLY	2.8
1	B	57	GLU	2.8
1	A	165	PHE	2.8
1	B	357	LEU	2.8
1	A	517	SER	2.7
1	B	5	SER	2.7
1	B	555	VAL	2.7
1	A	59	ALA	2.7
1	A	224	PRO	2.7
1	B	168	CYS	2.7
1	A	86	GLU	2.7
1	B	573	LYS	2.7
1	A	559	CYS	2.6
1	A	473	VAL	2.6
1	B	115	LEU	2.6
1	B	110	PRO	2.6
1	B	579	SER	2.6
1	B	81	ARG	2.6
1	B	170	GLN	2.6
1	A	555	VAL	2.6
1	B	300	ALA	2.6
1	B	271	ILE	2.6
1	B	560	LYS	2.6
1	B	95	GLU	2.5
1	B	501	GLU	2.5
1	B	335	ALA	2.5
1	B	392	CYS	2.5
1	B	565	GLU	2.5
1	A	279	CYS	2.5
1	A	562	ASP	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	53	CYS	2.5
1	A	5	SER	2.5
1	A	80	LEU	2.5
1	A	110	PRO	2.5
1	B	54	VAL	2.5
1	B	120	VAL	2.5
1	A	124	CYS	2.5
1	B	319	TYR	2.4
1	A	572	GLY	2.4
1	B	80	LEU	2.4
1	A	509	PHE	2.4
1	A	92	ALA	2.4
1	A	94	GLN	2.4
1	B	75	CYS	2.3
1	B	559	CYS	2.3
1	B	179	LEU	2.3
1	A	113	PRO	2.3
1	B	87	MET	2.3
1	B	178	LEU	2.3
1	B	63	ASP	2.3
1	B	59	ALA	2.3
1	A	512	ASP	2.3
1	A	171	ALA	2.3
1	A	554	PHE	2.3
1	A	570	GLU	2.3
1	B	510	HIS	2.2
1	B	166	THR	2.2
1	A	540	THR	2.2
1	A	535	HIS	2.2
1	B	542	GLU	2.2
1	A	502	PHE	2.2
1	A	278	CYS	2.2
1	B	50	ALA	2.2
1	B	427	SER	2.1
1	A	361	CYS	2.1
1	B	561	ALA	2.1
1	A	247	HIS	2.1
1	B	84	TYR	2.1
1	B	514	CYS	2.1
1	B	174	LYS	2.1
1	B	90	CYS	2.1
1	B	580	GLN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	365	ASP	2.1
1	A	564	LYS	2.1
1	B	564	LYS	2.1
1	A	65	SER	2.1
1	A	8	ALA	2.0
1	A	272	SER	2.0
1	B	408	LEU	2.0
1	B	34	CYS	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, 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	LLDF	B-factors(\AA^2)	Q<0.9
2	HLT	A	4003	7/7	0.75	0.57	16.32	84,86,87,95	7
2	HLT	B	4003	7/7	0.59	0.61	15.79	85,86,90,94	7
2	HLT	A	4001	7/7	0.83	0.36	4.59	73,73,74,81	7
2	HLT	B	4001	7/7	0.89	0.30	4.06	91,91,92,95	7
2	HLT	B	4002	7/7	0.78	0.28	3.98	75,76,77,81	7
2	HLT	A	4002	7/7	0.83	0.22	1.28	70,70,72,78	7

6.5 Other polymers [i](#)

There are no such residues in this entry.