



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:03 PM UTC

PDB ID : 1E7B / pdb_00001e7b
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

<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

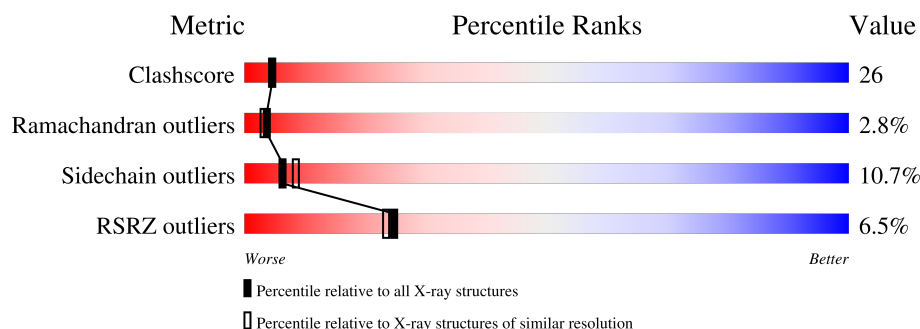
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (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 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	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	-
2	HLT	B	4001	-	-	X	-

2 Entry composition [i](#)

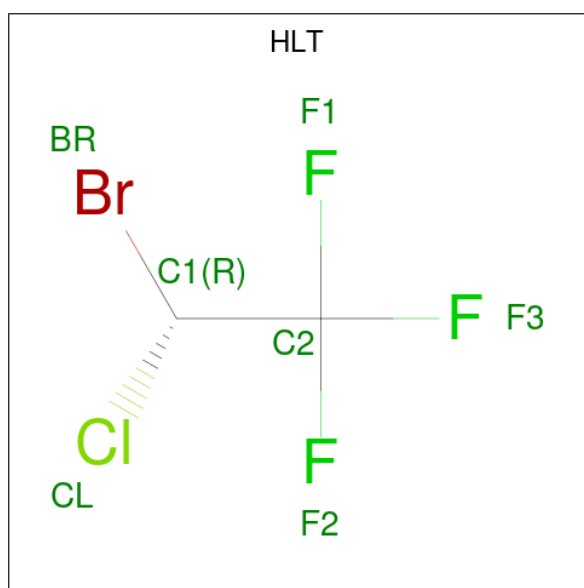
There are 3 unique types of molecules in this entry. The entry contains 8650 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: HLT) (formula: C₂HBrClF₃).



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		

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

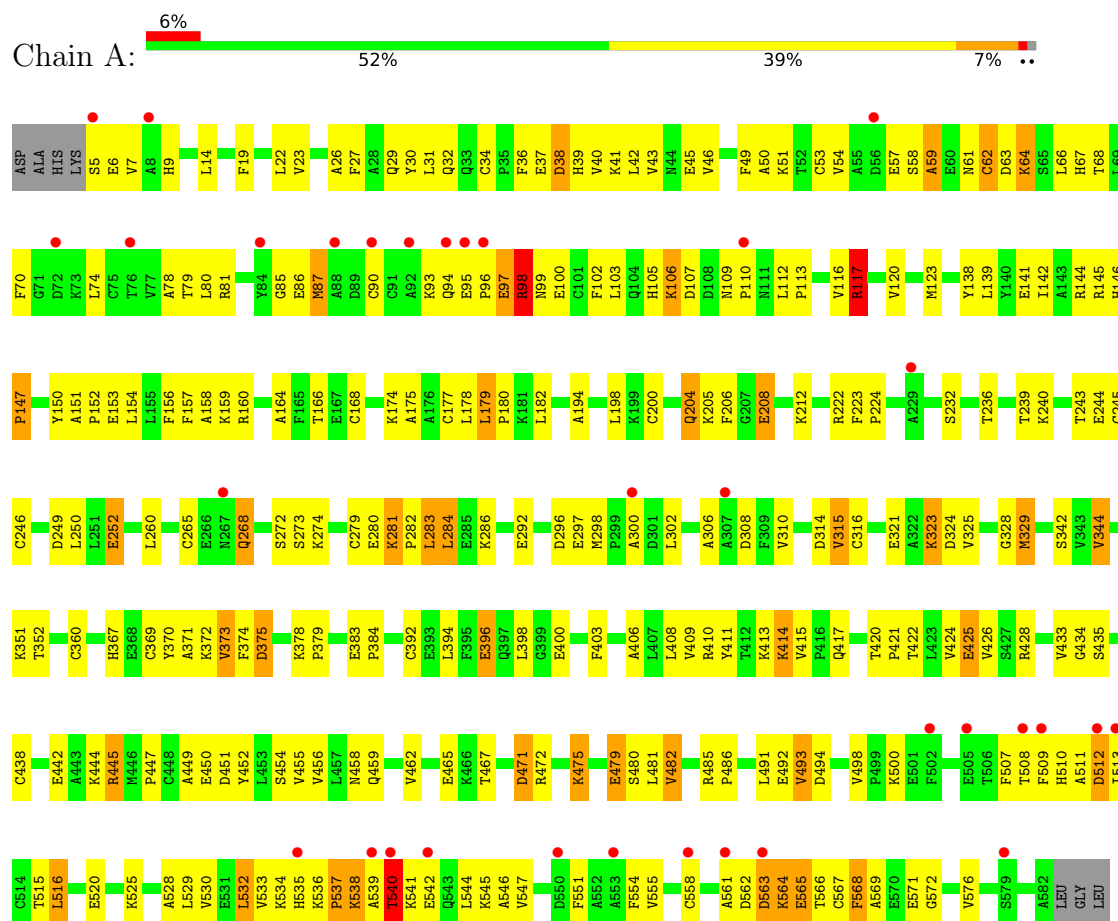
- Molecule 3 is water.

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

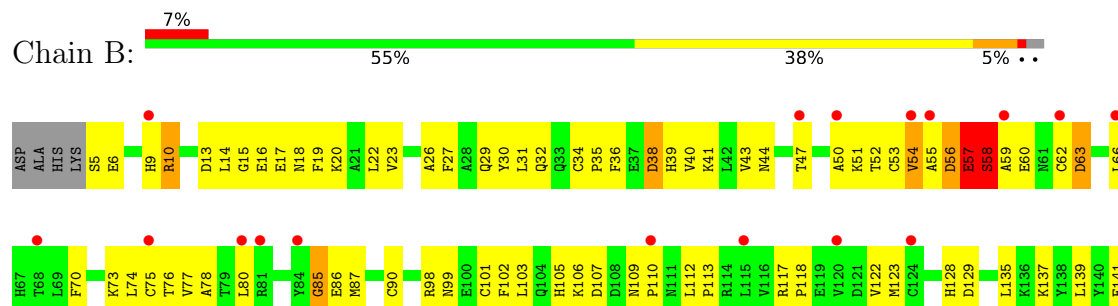
3 Residue-property plots

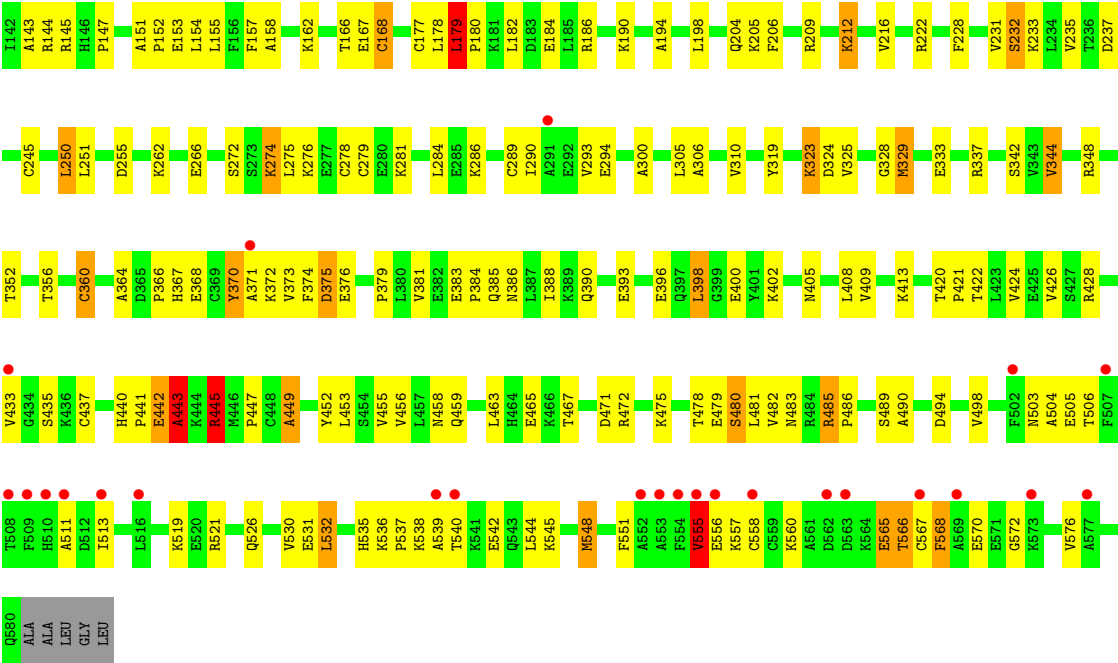
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 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	54.58Å 54.96Å 120.00Å 81.39° 90.79° 65.55°	Depositor
Resolution (Å)	17.00 – 2.38 17.00 – 2.38	Depositor EDS
% Data completeness (in resolution range)	96.0 (17.00-2.38) 95.8 (17.00-2.38)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 2.37Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.270 , 0.303 0.252 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	53.4	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 82.0	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	0.94	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, 0.333 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: 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	0.41	0/4388	0.99	19/5965 (0.3%)
1	B	0.40	0/4329	0.93	10/5892 (0.2%)
All	All	0.41	0/8717	0.96	29/11857 (0.2%)

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	ARG	N-CA-C	-10.48	99.17	112.90
1	A	542	GLU	N-CA-C	-9.32	98.46	113.19
1	A	117	ARG	CA-C-N	8.38	128.44	119.89
1	A	117	ARG	C-N-CA	8.38	128.44	119.89
1	B	443	ALA	N-CA-C	-8.23	93.28	110.80
1	B	542	GLU	N-CA-C	-8.19	103.42	113.50
1	A	106	LYS	N-CA-C	-7.58	99.06	110.28
1	B	539	ALA	N-CA-C	7.55	126.89	110.80
1	B	445	ARG	N-CA-C	7.48	119.08	111.07
1	B	449	ALA	N-CA-C	7.07	118.64	111.07
1	A	541	LYS	N-CA-C	-6.63	96.68	110.80
1	B	168	CYS	N-CA-C	6.37	118.22	111.28
1	A	449	ALA	N-CA-C	6.30	117.84	110.97
1	B	400	GLU	N-CA-C	6.29	117.80	111.07
1	A	564	LYS	N-CA-C	-6.21	97.56	110.80
1	A	540	THR	N-CA-C	-6.12	97.77	110.80
1	B	538	LYS	N-CA-C	5.93	123.43	110.80
1	A	563	ASP	N-CA-C	-5.91	103.14	110.41
1	A	510	HIS	N-CA-C	-5.77	100.39	109.50
1	A	373	VAL	N-CA-C	5.63	115.82	110.42
1	A	561	ALA	N-CA-C	-5.54	101.65	109.96
1	A	415	VAL	CA-C-N	5.51	125.60	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	415	VAL	C-N-CA	5.51	125.60	119.32
1	A	204	GLN	N-CA-C	5.47	117.05	111.14
1	A	400	GLU	N-CA-C	5.30	116.74	111.07
1	B	250	LEU	N-CA-C	5.29	117.05	111.28
1	B	478	THR	N-CA-C	5.23	118.82	112.23
1	A	445	ARG	N-CA-C	5.22	116.66	111.07
1	A	59	ALA	N-CA-C	5.20	121.88	110.80

There are no chirality outliers.

There are no planarity outliers.

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	4303	0	3992	238	0
1	B	4248	0	3880	192	0
2	A	21	0	0	2	0
2	B	21	0	0	3	0
3	A	30	0	0	2	0
3	B	27	0	0	1	0
All	All	8650	0	7872	430	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 26.

All (430) 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:87:MET:HE1	1:A:105:HIS:HB3	1.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:297:GLU:O	1:A:297:GLU:CA	2.29	0.81
1:B:39:HIS:O	1:B:43:VAL:HG23	1.80	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:HA	1:A:425:GLU:OE1	1.85	0.75
1:B:22:LEU:HD21	1:B:155:LEU:HD11	1.68	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:B:556:GLU:HG3	1:B:557:LYS:N	2.01	0.73
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:B:87:MET:HE1	1:B:105:HIS:HB3	1.72	0.72
1:A:110:PRO:C	1:A:112:LEU:H	1.96	0.72
1:A:323:LYS:HG3	1:A:324:ASP:N	2.04	0.72
1:A:87:MET:HE1	1:A:105:HIS:CB	2.17	0.71
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:120:VAL:HG21	1:A:175:ALA:HA	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:THR:CG2	1:A:544:LEU:HG	2.20	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:A:179:LEU:HB2	1:A:180:PRO:HD3	1.75	0.69
1:B:52:THR:HA	1:B:56:ASP:OD2	1.92	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:H	1:A:98:ARG:NH1	1.87	0.68
1:A:325:VAL:HG12	1:A:329:MET:HE2	1.75	0.67
1:A:107:ASP:O	1:A:147:PRO:HG2	1.94	0.67
1:B:34:CYS:HB3	1:B:39:HIS:HE2	1.61	0.66
1:B:449:ALA:O	1:B:453:LEU:HG	1.95	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:118:PRO:HD2	1:B:123:MET:HE3	1.77	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
1:A:106:LYS:HD3	1:A:147:PRO:HB3	1.78	0.64
1:A:472:ARG:NH1	1:A:494:ASP:HA	2.13	0.64
1:A:471:ASP:OD1	1:A:471:ASP:N	2.26	0.64
1:B:310:VAL:HG11	1:B:374:PHE:CE1	2.32	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:GLU:HB3	1:A:384:PRO:CD	2.29	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:205:LYS:HE3	1:A:465:GLU:OE2	2.00	0.61
1:A:297:GLU:CA	1:A:298:MET:N	2.63	0.61
1:A:178:LEU:O	1:A:179:LEU:C	2.43	0.60
1:A:433:VAL:HG22	1:A:452:TYR:CD2	2.36	0.60
1:B:90:CYS:O	1:B:98:ARG:HG3	2.01	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:31:LEU:HG	1:A:74:LEU:HD22	1.82	0.60
1:A:39:HIS:O	1:A:43:VAL:HG23	2.02	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:141:GLU:OE1	1:A:141:GLU:HA	2.03	0.59
1:A:249:ASP:HB3	1:A:252:GLU:CD	2.28	0.59
1:A:281:LYS:CB	1:A:282:PRO:HD2	2.33	0.59
1:A:564:LYS:C	1:A:566:THR:H	2.09	0.58
1:B:437:CYS:O	1:B:440:HIS:HB2	2.02	0.58
1:B:485:ARG:HB3	1:B:486:PRO:HD3	1.84	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
1:B:29:GLN:HG2	1:B:143:ALA:O	2.03	0.58
1:A:66:LEU:O	1:A:70:PHE:HD2	1.84	0.58
1:A:328:GLY:CA	2:A:4001:HLT:BR	3.06	0.58
1:B:370:TYR:CD1	1:B:370:TYR:C	2.81	0.57
1:B:212:LYS:O	1:B:216:VAL:HG23	2.03	0.57
1:A:370:TYR:CD1	1:A:370:TYR:C	2.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:138:TYR:CZ	1:A:142:ILE:HD11	2.41	0.56
1:A:511:ALA:HA	1:A:568:PHE:CD2	2.40	0.56
1:A:99:ASN:HA	1:A:102:PHE:HD2	1.71	0.55
1:B:19:PHE:CD1	1:B:19:PHE:C	2.84	0.55
1:A:38:ASP:N	1:A:38:ASP:OD1	2.38	0.55
1:B:504:ALA:C	1:B:506:THR:H	2.13	0.55
1:A:156:PHE:CE1	1:A:160:ARG:HD2	2.42	0.55
1:A:297:GLU:O	1:A:298:MET:HA	2.06	0.55
1:B:408:LEU:HD11	1:B:526:GLN:HB3	1.89	0.54
1:A:38:ASP:O	1:A:42:LEU:HG	2.08	0.54
1:B:306:ALA:CA	1:B:310:VAL:HG22	2.37	0.54
1:B:405:ASN:O	1:B:409:VAL:HG23	2.07	0.54
1:A:49:PHE:CD1	1:A:49:PHE:C	2.85	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:145:ARG:O	1:A:146:HIS:HD2	1.89	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:B:370:TYR:C	1:B:370:TYR:HD1	2.15	0.54
1:A:408:LEU:HD21	1:A:530:VAL:HG23	1.90	0.54
1:A:168:CYS:SG	1:A:177:CYS:C	2.91	0.54
1:A:564:LYS:C	1:A:566:THR:N	2.65	0.54
1:B:383:GLU:HB3	1:B:384:PRO:CD	2.35	0.54
1:A:32:GLN:NE2	1:A:147:PRO:HG3	2.23	0.54
1:A:452:TYR:O	1:A:456:VAL:HG23	2.07	0.54
1:B:98:ARG:O	1:B:101:CYS:HB3	2.08	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
1:A:281:LYS:CB	1:A:282:PRO:CD	2.85	0.53
1:A:533:VAL:HG12	1:A:533:VAL:O	2.09	0.53
1:B:54:VAL:HG12	1:B:55:ALA:N	2.23	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:HD1	1:A:49:PHE:O	1.91	0.53
1:A:314:ASP:O	1:A:315:VAL:C	2.52	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:49:PHE:C	1:A:49:PHE:HD1	2.17	0.52
1:A:23:VAL:HG13	1:A:70:PHE:HE1	1.73	0.52
1:B:565:GLU:O	1:B:565:GLU:HG3	2.08	0.52
1:A:351:LYS:HD3	3:A:2016:HOH:O	2.08	0.52
1:B:348:ARG:HG3	1:B:482:VAL:HG12	1.90	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:5:SER:HA	1:A:62:CYS:O	2.10	0.52
1:A:30:TYR:HE1	1:A:103:LEU:HD23	1.75	0.52
1:A:110:PRO:C	1:A:112:LEU:N	2.64	0.52
1:A:41:LYS:O	1:A:45:GLU:HG3	2.09	0.52
1:A:507:PHE:CD1	1:A:509:PHE:CE2	2.98	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:A:563:ASP:C	1:A:564:LYS:O	2.49	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:356:THR:O	1:B:360:CYS:HB2	2.11	0.51
1:B:558:CYS:SG	1:B:568:PHE:N	2.83	0.51
1:B:558:CYS:SG	1:B:567:CYS:C	2.94	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:A:279:CYS:HA	1:A:286:LYS:CD	2.38	0.51
1:A:342:SER:HA	1:A:447:PRO:HA	1.93	0.51
1:A:373:VAL:HG13	1:A:374:PHE:CD1	2.46	0.51
1:B:10:ARG:NH1	1:B:255:ASP:OD2	2.44	0.51
1:B:23:VAL:O	1:B:27:PHE:CD1	2.64	0.51
1:B:504:ALA:C	1:B:506:THR:N	2.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:344:VAL:HG12	1:A:482:VAL:HG13	1.93	0.50
1:B:118:PRO:HB2	1:B:122:VAL:HB	1.92	0.50
1:A:6:GLU:O	1:A:9:HIS:HB3	2.10	0.50
1:B:441:PRO:O	1:B:442:GLU:C	2.52	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: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: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:36:PHE:O	1:A:40:VAL:HG23	2.13	0.49
1:A:538:LYS:O	1:A:539:ALA:C	2.55	0.49
1:B:51:LYS:C	1:B:53:CYS:H	2.20	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:A:179:LEU:O	1:A:180:PRO:C	2.56	0.48
1:B:328:GLY:HA2	2:B:4001:HLT:BR	2.69	0.48
1:A:19:PHE:CD1	1:A:19:PHE:C	2.91	0.48
1:B:386:ASN:O	1:B:390:GLN:HB2	2.14	0.48
1:B:558:CYS:HB3	1:B:568:PHE:CD2	2.48	0.48
1:A:179:LEU:HB2	1:A:180:PRO:CD	2.43	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: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:B:32:GLN:NE2	1:B:110:PRO:HG3	2.28	0.48
1:B:279:CYS:HA	1:B:286:LYS:CD	2.43	0.48
1:A:61:ASN:C	1:A:63:ASP:N	2.69	0.48
1:A:373:VAL:HG13	1:A:374:PHE:HD1	1.78	0.48
1:A:61:ASN:C	1:A:63:ASP:H	2.21	0.48
1:A:360:CYS:SG	1:A:369:CYS:C	2.97	0.48
1:A:475:LYS:O	1:A:479:GLU:HB2	2.13	0.48
1:A:509:PHE:CZ	1:A:551:PHE:CE1	3.01	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:GLU:O	1:A:96:PRO:C	2.57	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:29:GLN:HG2	1:A:147:PRO:HA	1.95	0.47
1:A:51:LYS:HA	1:A:54:VAL:CG2	2.45	0.47
1:B:373:VAL:C	1:B:375:ASP:H	2.21	0.47
1:B:503:ASN:OD1	1:B:504:ALA:N	2.47	0.47
1:A:78:ALA:C	1:A:80:LEU:H	2.21	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:A:41:LYS:HE3	1:A:42:LEU:CD2	2.45	0.47
1:B:409:VAL:CG1	1:B:413:LYS:HE3	2.39	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:168:CYS:SG	1:B:177:CYS:C	2.98	0.47
1:B:178:LEU:HG	1:B:182:LEU:HG	1.96	0.47
1:B:485:ARG:O	1:B:486:PRO:C	2.58	0.47
1:A:223:PHE:CD1	1:A:272:SER:HB2	2.50	0.46
1:A:425:GLU:OE1	1:A:425:GLU:CA	2.60	0.46
1:A:492:GLU:O	1:A:493:VAL:C	2.57	0.46
1:B:178:LEU:O	1:B:179:LEU:C	2.58	0.46
1:B:206:PHE:CE2	1:B:481:LEU:HD13	2.51	0.46
1:B:364:ALA:O	1:B:366:PRO:HD3	2.14	0.46
1:B:572:GLY:O	1:B:576:VAL:HG23	2.15	0.46
1:A:417:GLN:CD	1:A:417:GLN:H	2.23	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:A:222:ARG:C	1:A:224:PRO:HD3	2.40	0.46
1:B:531:GLU:O	1:B:535:HIS:CD2	2.61	0.46
1:B:373:VAL:C	1:B:375:ASP:N	2.73	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:370:TYR:C	1:A:370:TYR:HD1	2.22	0.46
1:A:403:PHE:O	1:A:406:ALA:HB3	2.16	0.46
1:B:63:ASP:OD1	1:B:63:ASP:O	2.34	0.46
1:B:376:GLU:O	1:B:379:PRO:HD2	2.15	0.46
1:B:472:ARG:NH1	1:B:494:ASP:CB	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:109:ASN:O	1:B:110:PRO:C	2.58	0.46
1:A:459:GLN:O	1:A:462:VAL:HG22	2.16	0.46
1:A:507:PHE:CZ	1:A:576:VAL:HG22	2.48	0.46
1:B:44:ASN:HA	1:B:47:THR:HG22	1.98	0.46
1:B:137:LYS:O	1:B:141:GLU:HG2	2.16	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:563:ASP:O	1:A:564:LYS:C	2.58	0.46
1:A:310:VAL:O	1:A:370:TYR:HE1	1.98	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:A:90:CYS:HA	1:A:93:LYS:HG3	1.98	0.45
1:A:117:ARG:CD	1:A:123:MET:HE1	2.47	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: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:81:ARG:CA	1:A:85:GLY:HA2	2.47	0.45
1:A:554:PHE:CZ	1:A:568:PHE:HD1	2.35	0.45
1:A:98:ARG:HG2	1:A:99:ASN:N	2.30	0.45
1:A:120:VAL:HG21	1:A:175:ALA:CA	2.44	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:351:LYS:CD	3:A:2016:HOH:O	2.62	0.45
1:B:85:GLY:C	1:B:87:MET:H	2.25	0.45
1:B:141:GLU:OE1	1:B:144:ARG:HD3	2.16	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:492:GLU:HG3	1:A:493:VAL:H	1.81	0.44
1:B:128:HIS:O	1:B:129:ASP:C	2.60	0.44
1:A:67:HIS:CE1	1:A:99:ASN:HD21	2.35	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:456:VAL:O	1:B:459:GLN:HB3	2.17	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:61:ASN:O	1:A:63:ASP:N	2.50	0.44

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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:566:THR:O	1:A:567:CYS:C	2.60	0.44
1:A:566:THR:O	1:A:569:ALA:N	2.48	0.44
1:B:70:PHE:N	1:B:70:PHE:CD1	2.86	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:B:112:LEU:O	1:B:113:PRO:C	2.60	0.44
1:A:14:LEU:HD13	1:A:22:LEU:CD1	2.42	0.44
1:A:204:GLN:HE21	1:A:246:CYS:HB3	1.82	0.44
1:B:141:GLU:OE1	1:B:141:GLU:HA	2.18	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:17:GLU:O	1:B:18:ASN:C	2.61	0.43
1:B:30:TYR:CE1	1:B:103:LEU:HD23	2.53	0.43
1:B:536:LYS:O	1:B:537:PRO:C	2.61	0.43
1:A:512:ASP:O	1:A:515:THR:HG22	2.19	0.43
1:B:9:HIS:O	1:B:13:ASP:HB2	2.18	0.43
1:A:78:ALA:C	1:A:80:LEU:N	2.76	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:274:LYS:HE3	1:A:296:ASP:HA	2.01	0.43
1:A:451:ASP:O	1:A:454:SER:HB2	2.18	0.43
1:B:483:ASN:C	1:B:486:PRO:HD2	2.44	0.43
1:B:209:ARG:CG	2:B:4001:HLT:F2	2.56	0.43
1:B:422:THR:HG23	1:B:463:LEU:CD1	2.49	0.43
1:A:509:PHE:CE1	1:A:551:PHE:HZ	2.36	0.43
1:A:511:ALA:C	1:A:513:ILE:H	2.26	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:95:GLU:O	1:A:97:GLU:N	2.52	0.42
1:B:66:LEU:HD22	1:B:251:LEU:HD12	2.00	0.42
1:A:194:ALA:HB1	1:A:455:VAL:CG1	2.50	0.42
1:A:240:LYS:HE2	1:A:244:GLU:OE2	2.19	0.42
1:A:536:LYS:N	1:A:537:PRO:HD3	2.33	0.42
1:B:56:ASP:OD1	1:B:56:ASP:N	2.52	0.42
1:B:75:CYS:HA	1:B:78:ALA:HB3	2.01	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:B:442:GLU:HA	1:B:445:ARG:HD2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:PHE:O	1:B:232:SER:OG	2.35	0.42
1:B:374:PHE:CD1	1:B:374:PHE:N	2.87	0.42
1:B:532:LEU:HD23	1:B:532:LEU:HA	1.88	0.42
1:A:566:THR:C	1:A:568:PHE:N	2.75	0.42
1:A:408:LEU:HD11	1:A:530:VAL:CG2	2.49	0.42
1:B:179:LEU:HB2	1:B:180:PRO:HD3	2.01	0.42
1:A:100:GLU:HA	1:A:100:GLU:OE1	2.20	0.42
1:B:275:LEU:O	1:B:276:LYS:C	2.62	0.42
1:B:30:TYR:OH	1:B:103:LEU:HD21	2.20	0.42
1:B:329:MET:HE3	1:B:329:MET:HB2	1.94	0.42
1:A:420:THR:HG23	1:A:530:VAL:HG11	2.02	0.42
1:B:30:TYR:HD1	1:B:30:TYR:HA	1.74	0.42
1:B:57:GLU:HB3	1:B:58:SER:H	1.52	0.42
1:B:70:PHE:N	1:B:70:PHE:HD1	2.17	0.42
1:A:99:ASN:O	1:A:103:LEU:HG	2.19	0.42
1:B:519:LYS:C	1:B:521:ARG:N	2.78	0.42
1:A:535:HIS:O	1:A:535:HIS:ND1	2.52	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:34:CYS:HA	1:B:35:PRO:HD3	1.90	0.41
1:B:78:ALA:C	1:B:80:LEU:H	2.27	0.41
1:B:278:CYS:HB3	1:B:289:CYS:HB3	1.91	0.41
1:B:374:PHE:HD1	1:B:374:PHE:N	2.18	0.41
1:B:408:LEU:HD23	1:B:408:LEU:HA	1.94	0.41
1:A:110:PRO:HB3	1:A:112:LEU:HG	2.01	0.41
1:A:308:ASP:OD1	1:A:308:ASP:N	2.53	0.41
1:A:97:GLU:CB	1:A:100:GLU:CG	2.98	0.41
1:B:85:GLY:C	1:B:87:MET:N	2.79	0.41
1:B:18:ASN:O	1:B:22:LEU:HG	2.21	0.41
1:A:302:LEU:HD23	1:A:302:LEU:HA	1.95	0.41
1:B:29:GLN:HG3	1:B:143:ALA:HB1	2.01	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:139:LEU:HD22	1:A:154:LEU:HG	2.03	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:394:LEU:O	1:A:398:LEU:HG	2.20	0.41
1:B:366:PRO:C	1:B:368:GLU:N	2.77	0.41
1:B:472:ARG:NH1	1:B:494:ASP:HB2	2.36	0.41
1:B:511:ALA:C	1:B:513:ILE:H	2.27	0.41
1:A:344:VAL:HG23	1:A:450:GLU:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:TYR:HA	1:A:414:LYS:HD3	2.01	0.41
1:B:555:VAL:O	1:B:556:GLU:C	2.63	0.41
1:B:32:GLN:HE21	1:B:110:PRO:HG2	1.86	0.41
1:B:408:LEU:HD22	1:B:530:VAL:CG2	2.51	0.41
1:A:95:GLU:C	1:A:97:GLU:N	2.79	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:B:519:LYS:C	1:B:521:ARG:H	2.28	0.41
1:A:378:LYS:HB3	1:A:379:PRO:CD	2.46	0.40
1:A:545:LYS:O	1:A:546:ALA:C	2.62	0.40
1:A:507:PHE:CD1	1:A:509:PHE:CD2	3.07	0.40
1:B:29:GLN:HG2	1:B:147:PRO:HA	2.02	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%)	3	2
1	B	574/585 (98%)	493 (86%)	67 (12%)	14 (2%)	4	4
All	All	1148/1170 (98%)	991 (86%)	125 (11%)	32 (3%)	4	3

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

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Mol	Chain	Res	Type
1	B	57	GLU
1	B	58	SER
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%)	375 (88%)	50 (12%)	5	6
1	B	415/511 (81%)	375 (90%)	40 (10%)	8	11
All	All	840/1022 (82%)	750 (89%)	90 (11%)	6	8

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	GLU
1	A	38	ASP
1	A	64	LYS
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	159	LYS
1	A	166	THR
1	A	174	LYS
1	A	208	GLU
1	A	232	SER
1	A	236	THR
1	A	245	CYS
1	A	252	GLU
1	A	260	LEU
1	A	268	GLN
1	A	273	SER
1	A	280	GLU
1	A	281	LYS
1	A	283	LEU
1	A	284	LEU
1	A	292	GLU
1	A	323	LYS
1	A	329	MET
1	A	344	VAL
1	A	352	THR
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	475	LYS
1	A	480	SER

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Mol	Chain	Res	Type
1	A	482	VAL
1	A	493	VAL
1	A	498	VAL
1	A	508	THR
1	A	516	LEU
1	A	532	LEU
1	A	555	VAL
1	A	568	PHE
1	B	10	ARG
1	B	38	ASP
1	B	56	ASP
1	B	57	GLU
1	B	58	SER
1	B	63	ASP
1	B	166	THR
1	B	167	GLU
1	B	179	LEU
1	B	184	GLU
1	B	204	GLN
1	B	212	LYS
1	B	222	ARG
1	B	232	SER
1	B	245	CYS
1	B	274	LYS
1	B	281	LYS
1	B	284	LEU
1	B	305	LEU
1	B	323	LYS
1	B	329	MET
1	B	344	VAL
1	B	352	THR
1	B	360	CYS
1	B	370	TYR
1	B	375	ASP
1	B	398	LEU
1	B	435	SER
1	B	445	ARG
1	B	467	THR
1	B	471	ASP
1	B	480	SER
1	B	485	ARG
1	B	489	SER

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Mol	Chain	Res	Type
1	B	498	VAL
1	B	532	LEU
1	B	548	MET
1	B	555	VAL
1	B	566	THR
1	B	568	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	HIS
1	A	99	ASN
1	A	109	ASN
1	A	146	HIS
1	A	204	GLN
1	A	295	ASN
1	A	385	GLN
1	A	429	ASN
1	A	458	ASN
1	A	459	GLN
1	A	483	ASN
1	A	522	GLN
1	B	196	GLN
1	B	204	GLN
1	B	221	GLN
1	B	267	ASN
1	B	318	ASN
1	B	386	ASN
1	B	535	HIS

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](#)

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	B	4001	-	4,6,6	1.33	1 (25%)	3,9,9	1.29	0
2	HLT	A	4003	-	4,6,6	1.03	1 (25%)	3,9,9	1.19	0
2	HLT	A	4001	-	4,6,6	1.48	1 (25%)	3,9,9	1.32	0
2	HLT	A	4002	-	4,6,6	1.00	0	3,9,9	1.22	0
2	HLT	B	4003	-	4,6,6	1.15	1 (25%)	3,9,9	1.34	0
2	HLT	B	4002	-	4,6,6	1.07	1 (25%)	3,9,9	1.31	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	B	4001	-	-	3/3/6/6	-
2	HLT	A	4003	-	-	0/3/6/6	-
2	HLT	A	4001	-	-	3/3/6/6	-
2	HLT	A	4002	-	-	0/3/6/6	-
2	HLT	B	4003	-	-	0/3/6/6	-
2	HLT	B	4002	-	-	0/3/6/6	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4001	HLT	BR-C1	-2.94	1.87	1.96
2	B	4001	HLT	BR-C1	-2.47	1.89	1.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4003	HLT	BR-C1	-2.30	1.89	1.96
2	B	4002	HLT	BR-C1	-2.09	1.90	1.96
2	A	4003	HLT	BR-C1	-2.04	1.90	1.96

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4001	HLT	CL-C1-C2-F1
2	A	4001	HLT	CL-C1-C2-F2
2	A	4001	HLT	CL-C1-C2-F3
2	B	4001	HLT	CL-C1-C2-F1
2	B	4001	HLT	CL-C1-C2-F2
2	B	4001	HLT	CL-C1-C2-F3

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	4001	HLT	3	0
2	A	4001	HLT	2	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%)	0.43	33 (5%) 29 28	25, 69, 132, 144	0
1	B	576/585 (98%)	0.57	42 (7%) 21 20	34, 78, 137, 150	0
All	All	1154/1170 (98%)	0.50	75 (6%) 25 23	25, 73, 135, 150	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	539	ALA	6.5
1	B	563	ASP	5.4
1	B	508	THR	5.3
1	B	516	LEU	4.6
1	B	573	LYS	4.6
1	B	562	ASP	4.5
1	A	505	GLU	4.5
1	B	502	PHE	4.2
1	B	539	ALA	4.0
1	A	56	ASP	3.9
1	A	558	CYS	3.5
1	B	558	CYS	3.4
1	A	95	GLU	3.4
1	B	540	THR	3.4
1	A	229	ALA	3.4
1	B	569	ALA	3.3
1	A	110	PRO	3.2
1	B	555	VAL	3.2
1	B	59	ALA	3.2
1	A	502	PHE	3.1
1	A	542	GLU	3.1
1	B	81	ARG	3.1
1	A	84	TYR	3.1
1	A	96	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	76	THR	3.1
1	B	68	THR	3.1
1	B	552	ALA	3.0
1	A	72	ASP	3.0
1	B	507	PHE	2.9
1	A	8	ALA	2.9
1	B	554	PHE	2.9
1	A	540	THR	2.9
1	A	563	ASP	2.9
1	B	50	ALA	2.8
1	A	92	ALA	2.8
1	B	110	PRO	2.8
1	B	54	VAL	2.7
1	B	553	ALA	2.7
1	B	567	CYS	2.7
1	B	124	CYS	2.7
1	B	80	LEU	2.6
1	A	88	ALA	2.5
1	A	513	ILE	2.5
1	B	115	LEU	2.5
1	B	513	ILE	2.5
1	A	550	ASP	2.5
1	A	553	ALA	2.5
1	B	55	ALA	2.5
1	B	510	HIS	2.5
1	B	511	ALA	2.5
1	A	561	ALA	2.4
1	B	433	VAL	2.4
1	A	579	SER	2.4
1	B	62	CYS	2.4
1	A	508	THR	2.3
1	B	84	TYR	2.3
1	B	120	VAL	2.3
1	B	509	PHE	2.3
1	B	556	GLU	2.3
1	A	267	ASN	2.3
1	A	307	ALA	2.3
1	B	577	ALA	2.3
1	B	47	THR	2.3
1	B	66	LEU	2.2
1	A	94	GLN	2.2
1	B	9	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	291	ALA	2.2
1	A	512	ASP	2.2
1	A	90	CYS	2.2
1	A	300	ALA	2.1
1	B	371	ALA	2.1
1	A	509	PHE	2.1
1	A	5	SER	2.1
1	B	75	CYS	2.0
1	A	535	HIS	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	HLT	B	4003	7/7	0.55	0.20	85,86,90,94	7
2	HLT	A	4003	7/7	0.74	0.15	84,86,87,95	7
2	HLT	B	4002	7/7	0.78	0.13	75,76,77,81	7
2	HLT	A	4002	7/7	0.81	0.12	70,70,72,78	7
2	HLT	A	4001	7/7	0.89	0.16	73,73,74,81	7
2	HLT	B	4001	7/7	0.91	0.11	91,91,92,95	7

6.5 Other polymers [i](#)

There are no such residues in this entry.