Full wwPDB X-ray Structure Validation Report (i)

Dec 4, 2023 – 05:54 am 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

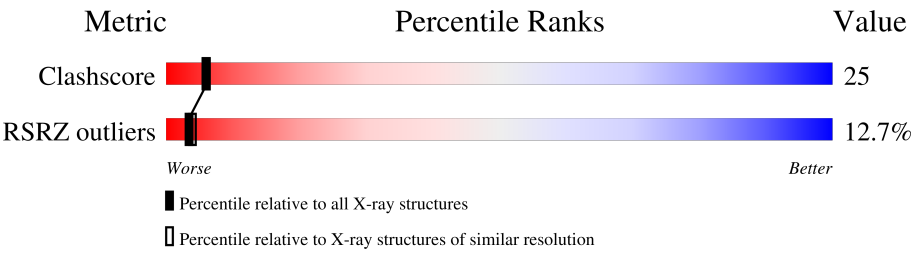
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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	141614	6082 (2.40-2.36)
RSRZ outliers	127900	5397 (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 <=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	11% 59% 39% •
1	B	585	14% 62% 36% •

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

2 Entry composition (i)

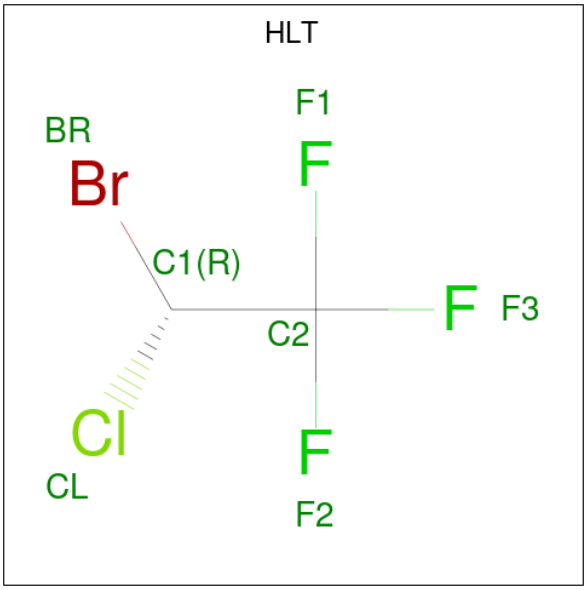
There are 3 unique types of molecules in this entry. The entry contains 8650 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	578	4303	2732	728	803	40	0	0	0
1	B	576	4248	2684	717	806	41	0	0	0

- 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
			Total	Br	C	Cl	F		
2	A	1	7	1	2	1	3	0	0
2	A	1	7	1	2	1	3	0	0
2	A	1	7	1	2	1	3	0	0
2	B	1	7	1	2	1	3	0	0

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

- Molecule 3 is water.

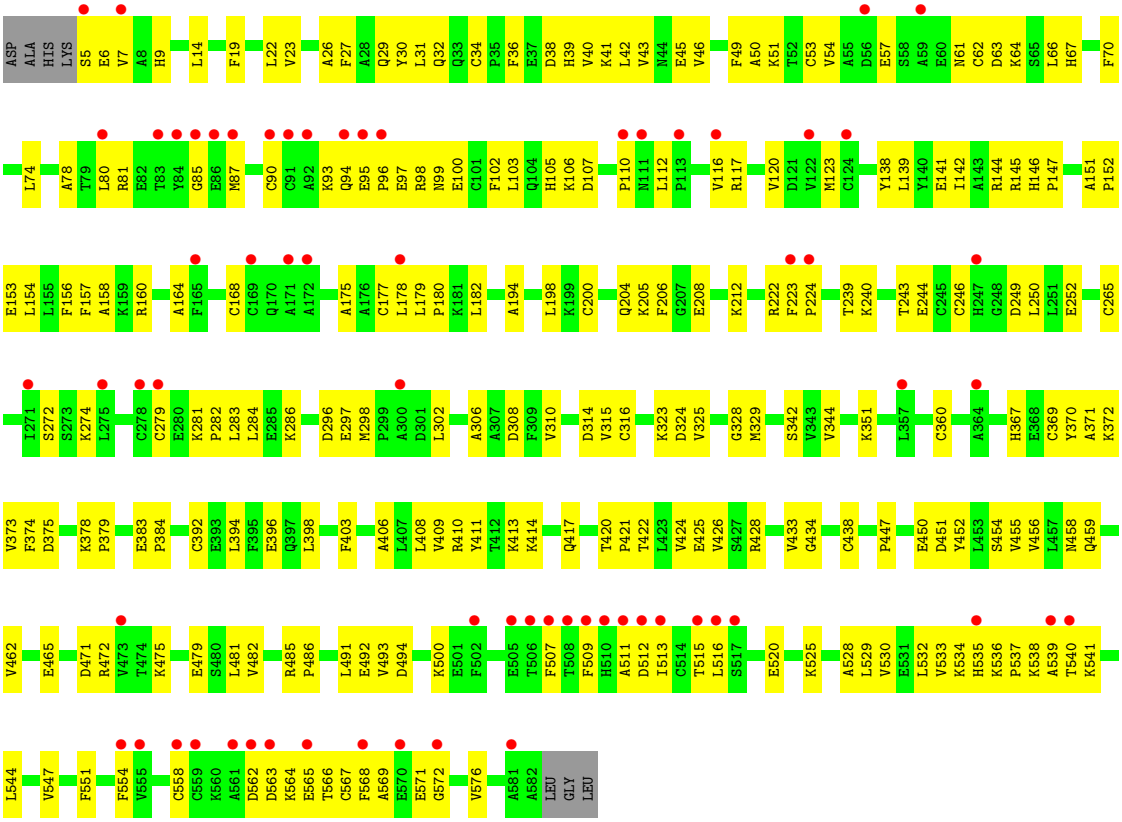
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	30	30	30	0	0
			Total	O		
3	B	27	27	27	0	0

3 Residue-property plots (i)

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.

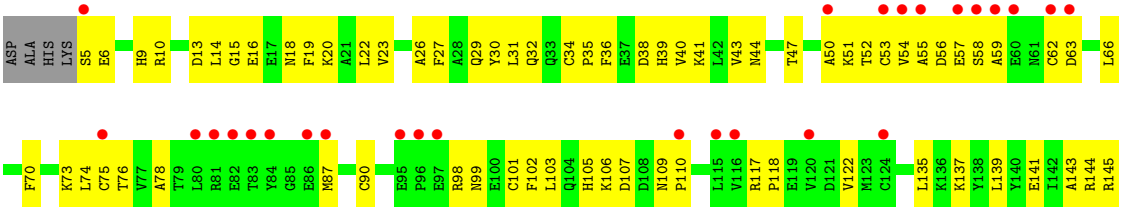
• Molecule 1: SERUM ALBUMIN

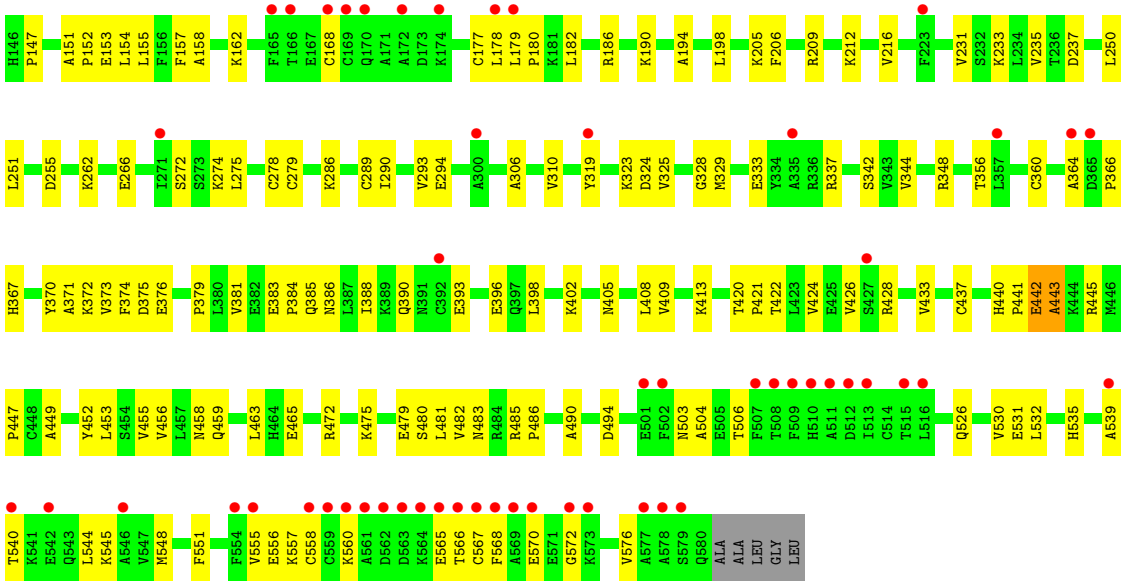
Chain A:



• Molecule 1: SERUM ALBUMIN

Chain B:




H146 P147 A151 P152 E153 L154 L155 F156 F157 A158 K162 F165 T166 E167 C168 C169 Q170 A171 A172 D173 K174 C177 L178 L179 P180 K181 L182 R186 K190 A194 L198 K205 F206 R209 K212 V216 F223 V231 S232 K233 L234 V235 T236 D237 L250
L251 D255 K262 E266 I271 S272 S273 K274 L275 C278 C279 K286 C289 I290 V293 E294 A300 A306 V310 Y319 K323 D324 V325 G328 M329 E333 Y334 A335 R336 R337 S342 V343 V344 R348 T356 L357 C360 A364 D365 P366
H367 Y370 A371 K372 V373 F374 D375 E376 P379 L380 V381 E382 E383 P384 Q385 N386 L387 I388 K389 Q390 N391 C392 E393 E396 Q397 L398 K402 N405 L408 V409 K413 T420 P421 T422 L423 V424 E425 V426 S427 R428 V433 C437 H440 P441 E442 A443 K444 R445 M446
P447 G448 A449 Y452 L453 S454 V455 V456 L457 N458 Q459 L463 H464 E465 R472 K475 E479 S480 L481 V482 N483 R484 R485 P486 A490 D494 E501 F502 N503 A504 E505 T506 F507 T508 F509 H510 A511 D512 I513 C514 T515 L516 Q526 V530 E531 L532 H535 A539
T540 K541 E542 Q543 L544 K545 A546 V547 M548 F551 F554 V555 E556 K557 C558 C559 K560 A561 D562 D563 K564 E565 T566 C567 F568 A569 E570 E571 G572 K573 V576 A577 A578 S579 Q580 ALA ALA LEU GLY LEU

4 Data and refinement statistics (i)

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 14.97 – 2.38	Depositor EDS
% Data completeness (in resolution range)	96.0 (17.00-2.38) 96.2 (14.97-2.38)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	3.03 (at 2.37Å)	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.	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)	0.29 , 81.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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	0.33	0/4379	0.58	1/5952 (0.0%)
1	B	0.34	1/4329 (0.0%)	0.54	2/5892 (0.0%)
All	All	0.34	1/8708 (0.0%)	0.56	3/11844 (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(^{o})	Ideal(^{o})
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

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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: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

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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:120:VAL:HG21	1:A:175:ALA:HA	1.73	0.70
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:281:LYS:CB	1:A:282:PRO:HD2	2.33	0.59
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

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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: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: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:A:178:LEU:O	1:A:179:LEU:C	2.43	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:A:38:ASP:N	1:A:38:ASP:OD1	2.38	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: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: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: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:A:249:ASP:HB3	1:A:252:GLU:CD	2.28	0.54
1:A:408:LEU:HD21	1:A:530:VAL:HG23	1.90	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:A:564:LYS:C	1:A:566:THR:H	2.09	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

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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: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:B:370:TYR:CD1	1:B:370:TYR:C	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: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: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: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: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: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

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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: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: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:36:PHE:O	1:A:40:VAL:HG23	2.13	0.49
1:A:564:LYS:C	1:A:566:THR:N	2.65	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:A:168:CYS:SG	1:A:177:CYS: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: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: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
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

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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: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
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:A:51:LYS:HA	1:A:54:VAL:CG2	2.45	0.47
1:B:503:ASN:OD1	1:B:504:ALA:N	2.47	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: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:B:558:CYS:SG	1:B:567:CYS:C	2.94	0.47
1:A:42:LEU:O	1:A:46:VAL:HG23	2.15	0.47
1:A:563:ASP:C	1:A:564:LYS:O	2.49	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: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: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: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: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:504:ALA:C	1:B:506:THR:N	2.69	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:459:GLN:O	1:A:462:VAL:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:441:PRO:O	1:B:442:GLU:C	2.52	0.46
1:A:61:ASN:C	1:A:63:ASP:N	2.69	0.45
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:51:LYS:C	1:B:53:CYS:H	2.20	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: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: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: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:434:GLY:O	1:A:438:CYS:HB2	2.17	0.44
1:A:538:LYS:O	1:A:539:ALA:C	2.55	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: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:61:ASN:O	1:A:63:ASP:N	2.50	0.44
1:A:525:LYS:O	1:A:528:ALA:HB3	2.17	0.44
1:A:566:THR:O	1:A:569:ALA:N	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:325:VAL:HG12	1:A:329:MET:CE	2.47	0.44
1:A:420:THR:HG23	1:A:530:VAL:CG1	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:A:19:PHE:CD1	1:A:19:PHE:C	2.91	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:30:TYR:CE1	1:B:103:LEU:HD23	2.53	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:B:373:VAL:C	1:B:375:ASP:H	2.21	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:95:GLU:O	1:A:96:PRO:C	2.57	0.43
1:A:274:LYS:HE3	1:A:296:ASP:HA	2.01	0.43
1:A:360:CYS:SG	1:A:369:CYS:C	2.97	0.43
1:A:451:ASP:O	1:A:454:SER:HB2	2.18	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:B:272:SER:HB3	1:B:275:LEU:HG	2.01	0.43
1:A:78:ALA:C	1:A:80:LEU:H	2.21	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ASN:C	1:A:63:ASP:H	2.21	0.42
1:A:408:LEU:HD11	1:A:530:VAL:CG2	2.49	0.42
1:B:168:CYS:SG	1:B:177:CYS:C	2.98	0.42
1:B:179:LEU:HB2	1:B:180:PRO:HD3	2.01	0.42
1:B:531:GLU:OE1	1:B:531:GLU:HA	2.19	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:222:ARG:C	1:A:224:PRO:HD3	2.40	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:B:485:ARG:O	1:B:486:PRO:C	2.58	0.42
1:A:99:ASN:O	1:A:103:LEU:HG	2.19	0.42
1:A:492:GLU:O	1:A:493:VAL:C	2.57	0.42
1:B:178:LEU:O	1:B:179:LEU:C	2.58	0.42
1:A:417:GLN:CD	1:A:417:GLN:H	2.23	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:373:VAL:C	1:B:375:ASP:N	2.73	0.42
1:B:34:CYS:HA	1:B:35:PRO:HD3	1.90	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:370:TYR:C	1:A:370:TYR:HD1	2.22	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: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:472:ARG:NH1	1:B:494:ASP:HB2	2.36	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:A:563:ASP:O	1:A:564:LYS:C	2.58	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
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: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)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 monosaccharides 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	4002	-	4,6,6	0.95	0	3,9,9	1.27	0
2	HLT	B	4003	-	4,6,6	1.03	1 (25%)	3,9,9	1.30	0
2	HLT	A	4002	-	4,6,6	0.88	0	3,9,9	1.19	0
2	HLT	A	4003	-	4,6,6	0.92	0	3,9,9	1.16	0
2	HLT	A	4001	-	4,6,6	1.34	1 (25%)	3,9,9	1.29	0
2	HLT	B	4001	-	4,6,6	1.19	1 (25%)	3,9,9	1.25	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	4002	-	-	0/3/6/6	-
2	HLT	B	4003	-	-	0/3/6/6	-
2	HLT	A	4002	-	-	0/3/6/6	-
2	HLT	A	4003	-	-	0/3/6/6	-
2	HLT	A	4001	-	-	3/3/6/6	-
2	HLT	B	4001	-	-	3/3/6/6	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4001	HLT	BR-C1	-2.64	1.87	1.96
2	B	4001	HLT	BR-C1	-2.20	1.89	1.96
2	B	4003	HLT	BR-C1	-2.05	1.89	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.

3 monomers are involved in 6 short contacts:

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

6.1 Protein, DNA and RNA chains (i)

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%)	0.60	66 (11%)	5	5	25, 69, 132, 144	0
1	B	576/585 (98%)	0.73	81 (14%)	2	3	34, 78, 137, 150	0
All	All	1154/1170 (98%)	0.67	147 (12%)	3	4	25, 73, 135, 150	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	539	ALA	11.6
1	B	539	ALA	10.5
1	B	563	ASP	10.1
1	B	562	ASP	7.6
1	A	96	PRO	7.3
1	B	83	THR	7.2
1	A	506	THR	5.7
1	A	568	PHE	5.7
1	B	577	ALA	5.5
1	B	508	THR	5.3
1	A	85	GLY	5.3
1	B	364	ALA	5.2
1	B	507	PHE	5.1
1	B	165	PHE	5.0
1	A	300	ALA	5.0
1	A	513	ILE	4.9
1	B	116	VAL	4.8
1	B	558	CYS	4.6
1	A	505	GLU	4.6
1	B	515	THR	4.6
1	A	364	ALA	4.6
1	B	172	ALA	4.3
1	B	82	GLU	4.2
1	B	567	CYS	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	83	THR	4.1
1	B	540	THR	4.1
1	A	563	ASP	4.1
1	A	116	VAL	4.1
1	A	516	LEU	4.1
1	A	565	GLU	4.0
1	B	578	ALA	3.9
1	B	569	ALA	3.8
1	B	502	PHE	3.8
1	B	512	ASP	3.8
1	A	84	TYR	3.7
1	A	56	ASP	3.7
1	A	271	ILE	3.7
1	B	516	LEU	3.6
1	B	546	ALA	3.6
1	B	365	ASP	3.6
1	A	507	PHE	3.5
1	B	511	ALA	3.5
1	A	510	HIS	3.5
1	A	357	LEU	3.5
1	B	509	PHE	3.5
1	B	60	GLU	3.5
1	B	86	GLU	3.4
1	A	178	LEU	3.4
1	B	568	PHE	3.4
1	B	566	THR	3.4
1	A	511	ALA	3.4
1	A	581	ALA	3.4
1	B	169	CYS	3.3
1	A	223	PHE	3.3
1	A	87	MET	3.2
1	B	554	PHE	3.2
1	A	169	CYS	3.1
1	A	95	GLU	3.1
1	A	7	VAL	3.1
1	B	96	PRO	3.0
1	B	55	ALA	3.0
1	B	570	GLU	3.0
1	B	513	ILE	2.9
1	A	91	CYS	2.9
1	A	275	LEU	2.8
1	A	561	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	97	GLU	2.8
1	B	223	PHE	2.8
1	A	122	VAL	2.8
1	B	124	CYS	2.8
1	B	58	SER	2.8
1	A	515	THR	2.8
1	A	172	ALA	2.7
1	A	90	CYS	2.7
1	B	57	GLU	2.7
1	A	558	CYS	2.7
1	B	5	SER	2.7
1	A	111	ASN	2.7
1	A	508	THR	2.7
1	B	62	CYS	2.7
1	B	573	LYS	2.7
1	A	59	ALA	2.6
1	B	357	LEU	2.6
1	A	86	GLU	2.6
1	A	165	PHE	2.6
1	B	555	VAL	2.6
1	B	572	GLY	2.6
1	A	517	SER	2.6
1	A	224	PRO	2.6
1	B	168	CYS	2.5
1	B	81	ARG	2.5
1	B	300	ALA	2.5
1	B	579	SER	2.5
1	B	115	LEU	2.5
1	A	473	VAL	2.5
1	A	555	VAL	2.5
1	B	170	GLN	2.5
1	A	559	CYS	2.5
1	B	95	GLU	2.5
1	B	271	ILE	2.5
1	B	110	PRO	2.4
1	B	560	LYS	2.4
1	B	501	GLU	2.4
1	A	5	SER	2.4
1	B	565	GLU	2.4
1	A	562	ASP	2.4
1	A	279	CYS	2.4
1	B	392	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	110	PRO	2.3
1	B	335	ALA	2.3
1	B	120	VAL	2.3
1	B	319	TYR	2.3
1	A	80	LEU	2.3
1	B	54	VAL	2.3
1	B	559	CYS	2.3
1	A	124	CYS	2.3
1	B	53	CYS	2.3
1	A	509	PHE	2.3
1	A	94	GLN	2.3
1	B	80	LEU	2.2
1	A	92	ALA	2.2
1	A	572	GLY	2.2
1	A	570	GLU	2.2
1	B	178	LEU	2.2
1	B	87	MET	2.2
1	A	113	PRO	2.2
1	A	171	ALA	2.2
1	B	166	THR	2.2
1	B	63	ASP	2.2
1	B	75	CYS	2.2
1	A	512	ASP	2.2
1	B	179	LEU	2.1
1	B	59	ALA	2.1
1	A	278	CYS	2.1
1	A	535	HIS	2.1
1	B	510	HIS	2.1
1	B	84	TYR	2.1
1	A	502	PHE	2.1
1	A	554	PHE	2.1
1	B	542	GLU	2.1
1	A	540	THR	2.1
1	B	50	ALA	2.1
1	A	247	HIS	2.1
1	B	427	SER	2.0
1	B	561	ALA	2.0
1	B	174	LYS	2.0
1	B	564	LYS	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 monosaccharides 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(Å^2)	Q<0.9
2	HLT	B	4003	7/7	0.58	0.61	85,86,90,94	7
2	HLT	A	4003	7/7	0.74	0.57	84,86,87,95	7
2	HLT	B	4002	7/7	0.77	0.28	75,76,77,81	7
2	HLT	A	4002	7/7	0.82	0.23	70,70,72,78	7
2	HLT	A	4001	7/7	0.83	0.35	73,73,74,81	7
2	HLT	B	4001	7/7	0.89	0.30	91,91,92,95	7

6.5 Other polymers (i)

There are no such residues in this entry.