



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 05:13 pm BST

PDB ID : 1E7A
Title : Crystal structure of human serum albumin complexed with the general anesthetic propofol
Authors : Bhattacharya, A.A.; Curry, S.; Franks, N.P.
Deposited on : 2000-08-26
Resolution : 2.20 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

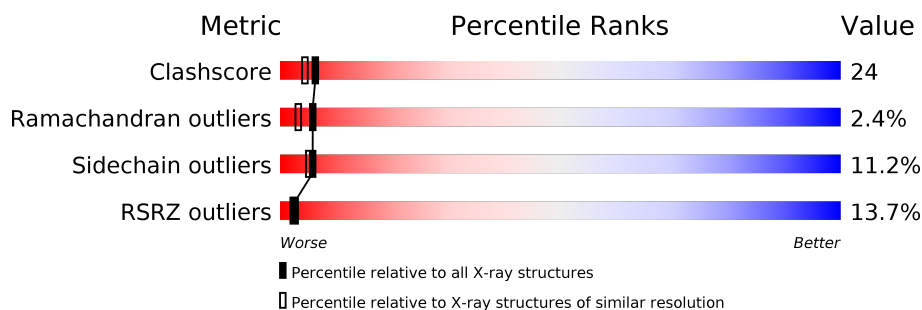
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 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	<div> <div>12%</div> <div>55%</div> <div>37%</div> <div>6% ..</div> </div>
1	B	585	<div> <div>15%</div> <div>58%</div> <div>36%</div> <div>5% ..</div> </div>

2 Entry composition [i](#)

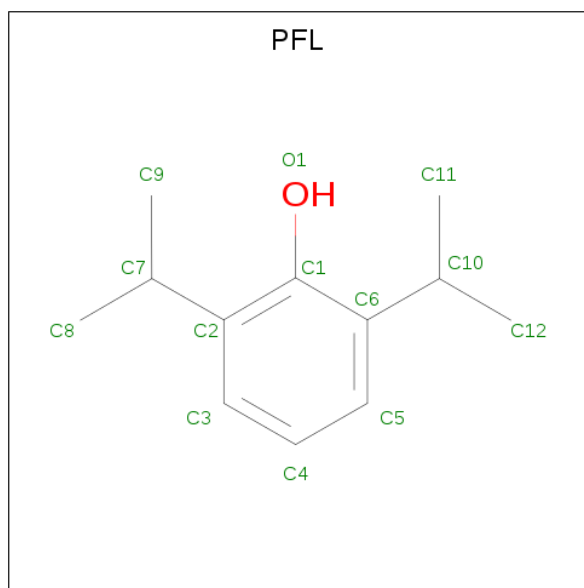
There are 3 unique types of molecules in this entry. The entry contains 9122 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			4470	2827	745	857	41			
1	B	578	Total	C	N	O	S	0	0	0
			4480	2832	747	860	41			

- Molecule 2 is 2,6-BIS(1-METHYLETHYL)PHENOL (three-letter code: PFL) (formula: $C_{12}H_{18}O$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	12	1		
2	A	1	Total	C	O	0	0
			13	12	1		
2	B	1	Total	C	O	0	0
			13	12	1		
2	B	1	Total	C	O	0	0
			13	12	1		

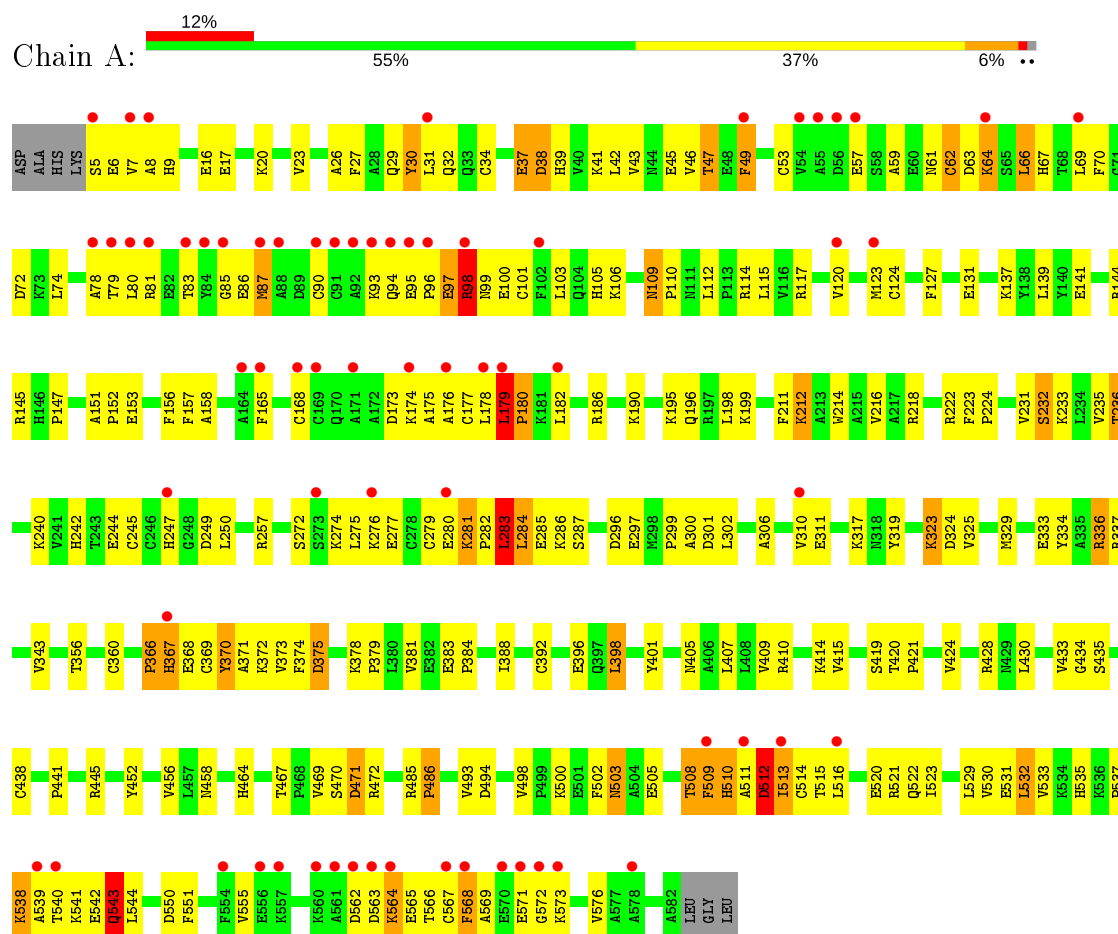
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	60	Total 60	O 60	0	0
3	B	60	Total 60	O 60	0	0

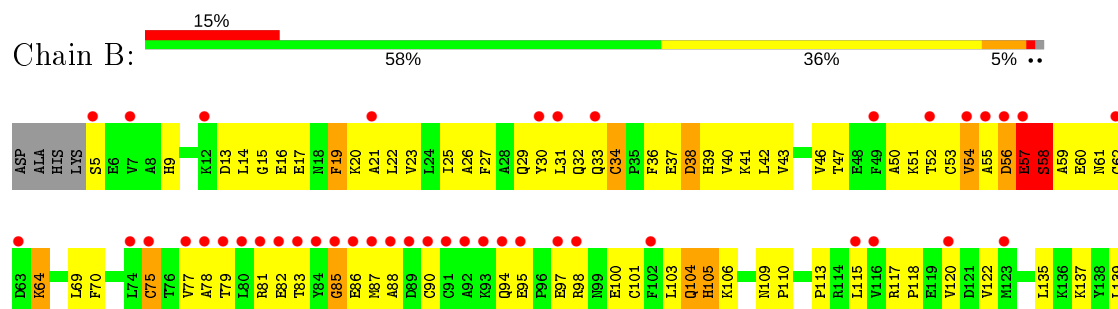
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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 ($\text{RSRZ} > 2$). 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	55.40 Å 55.61 Å 120.50 Å 81.11° 90.57° 65.50°	Depositor
Resolution (Å)	30.00 – 2.20 29.90 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.1 (30.00-2.20) 96.1 (29.90-2.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 2.20 Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.248 , 0.272 0.242 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 77.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9122	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.94% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.40	0/4558	0.61	3/6174 (0.0%)
1	B	0.35	0/4565	0.54	0/6178
All	All	0.38	0/9123	0.58	3/12352 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	509	PHE	N-CA-C	5.91	126.96	111.00
1	A	564	LYS	N-CA-C	-5.51	96.11	111.00
1	A	543	GLN	N-CA-C	-5.05	97.37	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	4470	0	4271	252	0
1	B	4480	0	4303	175	0
2	A	26	0	36	7	0
2	B	26	0	36	5	0
3	A	60	0	0	13	0
3	B	60	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9122	0	8646	428	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 24.

All (428) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:VAL:HG22	1:B:452:TYR:CD2	1.39	1.57
1:B:433:VAL:CG2	1:B:452:TYR:CD2	2.06	1.35
1:B:433:VAL:HG22	1:B:452:TYR:CE2	1.69	1.25
1:B:433:VAL:CG2	1:B:452:TYR:CE2	2.21	1.23
1:A:410:ARG:HD3	3:A:2035:HOH:O	1.08	1.21
1:A:540:THR:HG23	1:A:544:LEU:HD11	1.31	1.11
1:A:540:THR:HG23	1:A:544:LEU:CD1	1.84	1.07
1:A:97:GLU:C	1:A:99:ASN:H	1.50	1.07
1:A:94:GLN:O	1:A:98:ARG:HB3	1.57	1.04
1:A:540:THR:CG2	1:A:544:LEU:HD11	1.86	1.03
1:A:498:VAL:HG12	3:A:2056:HOH:O	1.61	0.97
1:A:152:PRO:HB2	1:A:257:ARG:HH11	1.28	0.96
1:B:433:VAL:CG2	1:B:452:TYR:HD2	1.65	0.95
1:A:485:ARG:HB3	1:A:486:PRO:HD3	1.46	0.95
1:A:222:ARG:HG3	3:A:2017:HOH:O	1.66	0.94
1:A:97:GLU:O	1:A:99:ASN:N	2.01	0.94
1:A:97:GLU:C	1:A:99:ASN:N	2.18	0.94
1:B:579:SER:CB	2:B:4002:PFL:O1	2.18	0.91
1:B:433:VAL:HG21	1:B:452:TYR:HD2	1.33	0.90
1:A:366:PRO:O	1:A:368:GLU:N	2.05	0.89
1:B:106:LYS:HD3	1:B:147:PRO:HB2	1.55	0.89
1:A:485:ARG:HB3	1:A:486:PRO:CD	2.03	0.88
1:B:433:VAL:HG23	1:B:452:TYR:CE2	2.09	0.87
1:B:579:SER:CB	2:B:4002:PFL:HO1	1.87	0.86
1:A:511:ALA:HB2	1:A:565:GLU:HB3	1.56	0.86
1:B:432:LYS:HE3	3:B:2037:HOH:O	1.74	0.86
1:A:367:HIS:O	1:A:371:ALA:HB2	1.76	0.85
1:A:283:LEU:HG	1:A:284:LEU:HD23	1.56	0.84
1:B:394:LEU:O	1:B:397:GLN:HG2	1.77	0.84
1:B:249:ASP:HB3	1:B:252:GLU:OE1	1.78	0.83
1:B:81:ARG:HE	1:B:88:ALA:HB3	1.42	0.83
1:A:42:LEU:O	1:A:46:VAL:HG23	1.77	0.83
1:A:106:LYS:HD3	1:A:147:PRO:HB2	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:GLN:HG2	1:B:147:PRO:HA	1.59	0.82
1:B:433:VAL:HG23	1:B:452:TYR:HE2	1.45	0.82
1:B:120:VAL:HG21	1:B:175:ALA:HA	1.61	0.81
1:A:98:ARG:CZ	1:A:99:ASN:HB2	2.11	0.80
1:A:378:LYS:HB3	1:A:379:PRO:HD3	1.62	0.80
1:A:282:PRO:HB2	1:A:285:GLU:OE1	1.82	0.80
1:A:540:THR:CG2	1:A:544:LEU:CD1	2.55	0.80
1:A:562:ASP:OD1	1:A:562:ASP:O	2.01	0.79
1:A:283:LEU:HG	1:A:284:LEU:N	1.97	0.79
1:B:579:SER:HB2	2:B:4002:PFL:O1	1.86	0.76
1:A:97:GLU:CB	1:A:100:GLU:HG2	2.16	0.75
1:A:151:ALA:HB3	1:A:152:PRO:HD3	1.68	0.75
1:B:199:LYS:HE3	3:B:2014:HOH:O	1.85	0.75
1:A:433:VAL:HG22	1:A:452:TYR:CE2	2.22	0.75
1:A:430:LEU:O	1:A:433:VAL:HG23	1.86	0.75
1:B:410:ARG:HD3	3:B:2039:HOH:O	1.88	0.74
1:B:100:GLU:O	1:B:104:GLN:HG3	1.88	0.74
1:B:571:GLU:OE1	1:B:574:LYS:HD2	1.88	0.73
1:B:433:VAL:HG21	1:B:452:TYR:CD2	2.09	0.73
1:B:571:GLU:HA	1:B:571:GLU:OE1	1.88	0.72
1:A:540:THR:HG23	1:A:544:LEU:CG	2.19	0.72
1:B:81:ARG:NE	1:B:88:ALA:HB3	2.05	0.71
1:A:424:VAL:O	1:A:428:ARG:HG3	1.90	0.71
1:A:306:ALA:HA	1:A:310:VAL:HG22	1.71	0.71
1:A:323:LYS:HG3	1:A:324:ASP:N	2.05	0.71
1:A:569:ALA:O	1:A:573:LYS:HG3	1.91	0.70
1:B:556:GLU:HG3	1:B:557:LYS:N	2.06	0.70
1:B:34:CYS:HB3	1:B:39:HIS:NE2	2.06	0.69
1:A:366:PRO:O	1:A:369:CYS:N	2.24	0.69
1:A:373:VAL:HG13	1:A:374:PHE:HD1	1.56	0.69
1:B:32:GLN:NE2	1:B:110:PRO:HG3	2.08	0.69
1:A:34:CYS:HB3	1:A:39:HIS:NE2	2.08	0.69
1:B:556:GLU:HG3	1:B:557:LYS:H	1.58	0.68
1:A:281:LYS:CB	1:A:282:PRO:HD2	2.23	0.68
1:A:433:VAL:HB	2:A:4001:PFL:HC7	1.76	0.68
1:A:281:LYS:HB2	1:A:282:PRO:HD2	1.76	0.67
1:B:384:PRO:O	1:B:388:ILE:HG12	1.94	0.67
1:B:135:LEU:HD11	1:B:162:LYS:HD3	1.75	0.67
1:A:98:ARG:HH11	1:A:98:ARG:N	1.93	0.67
1:A:120:VAL:HG21	1:A:175:ALA:HA	1.76	0.67
1:A:66:LEU:O	1:A:70:PHE:HD2	1.78	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:THR:HA	1:B:56:ASP:OD2	1.94	0.66
1:B:579:SER:HB3	2:B:4002:PFL:O1	1.93	0.66
1:B:279:CYS:HA	1:B:286:LYS:HD2	1.78	0.66
1:B:323:LYS:HE2	3:B:2027:HOH:O	1.95	0.66
1:B:424:VAL:O	1:B:428:ARG:HG3	1.96	0.66
1:A:153:GLU:O	1:A:157:PHE:HD1	1.80	0.65
1:A:372:LYS:O	1:A:375:ASP:HB2	1.96	0.65
1:A:464:HIS:CE1	1:A:469:VAL:H	2.14	0.65
1:A:433:VAL:HG22	1:A:452:TYR:CD2	2.30	0.65
1:A:279:CYS:HA	1:A:286:LYS:HD2	1.78	0.65
1:A:100:GLU:HA	1:A:100:GLU:OE1	1.96	0.65
1:A:26:ALA:HB2	1:A:250:LEU:HD12	1.78	0.65
1:B:15:GLY:O	1:B:19:PHE:HB3	1.97	0.65
1:A:67:HIS:HB3	1:A:98:ARG:HH21	1.61	0.65
1:A:66:LEU:HD13	1:A:66:LEU:N	2.12	0.64
1:B:26:ALA:HB2	1:B:250:LEU:HD12	1.80	0.64
1:B:39:HIS:O	1:B:43:VAL:HG23	1.97	0.64
1:A:31:LEU:HG	1:A:74:LEU:HD22	1.79	0.64
1:A:508:THR:HG23	1:A:510:HIS:CE1	2.31	0.64
1:B:323:LYS:HG3	1:B:324:ASP:N	2.10	0.64
1:A:392:CYS:O	1:A:396:GLU:HG3	1.97	0.63
1:A:509:PHE:O	1:A:568:PHE:CE1	2.51	0.63
1:A:541:LYS:O	1:A:542:GLU:HG3	1.98	0.63
1:A:564:LYS:O	1:A:566:THR:N	2.26	0.63
1:B:59:ALA:HB3	1:B:62:CYS:SG	2.38	0.63
1:A:39:HIS:O	1:A:43:VAL:HG23	1.99	0.63
1:B:383:GLU:HB3	1:B:384:PRO:HD3	1.79	0.63
1:B:90:CYS:O	1:B:98:ARG:HG3	2.00	0.62
1:A:511:ALA:HB2	1:A:565:GLU:CB	2.28	0.62
1:A:6:GLU:O	1:A:9:HIS:N	2.33	0.62
1:B:151:ALA:HB3	1:B:152:PRO:HD3	1.82	0.62
1:A:384:PRO:O	1:A:388:ILE:HG12	2.00	0.61
1:A:567:CYS:O	1:A:571:GLU:HB2	2.00	0.61
1:B:141:GLU:O	1:B:145:ARG:HG3	1.99	0.61
1:B:378:LYS:HB2	1:B:379:PRO:HD3	1.81	0.61
1:A:66:LEU:H	1:A:66:LEU:HD13	1.65	0.61
1:B:367:HIS:O	1:B:371:ALA:HB2	1.99	0.61
1:A:94:GLN:O	1:A:98:ARG:HD3	2.00	0.61
1:B:81:ARG:HE	1:B:88:ALA:CB	2.11	0.61
1:B:283:LEU:HG	1:B:284:LEU:N	2.14	0.61
1:A:565:GLU:OE1	1:A:565:GLU:HA	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:531:GLU:O	1:B:535:HIS:HD2	1.83	0.60
1:B:435:SER:O	1:B:439:LYS:HE2	2.01	0.60
1:A:471:ASP:N	1:A:471:ASP:OD1	2.30	0.60
1:A:177:CYS:SG	3:A:2009:HOH:O	2.56	0.60
1:A:532:LEU:HG	2:A:4002:PFL:H83	1.83	0.60
1:B:565:GLU:HG3	1:B:565:GLU:O	2.01	0.60
1:A:281:LYS:CB	1:A:282:PRO:CD	2.80	0.59
1:B:42:LEU:O	1:B:46:VAL:HG23	2.02	0.59
1:A:485:ARG:NE	1:A:486:PRO:HD3	2.18	0.59
1:A:152:PRO:HB2	1:A:257:ARG:NH1	2.10	0.59
1:A:41:LYS:NZ	1:A:45:GLU:OE2	2.30	0.59
1:A:97:GLU:CB	1:A:100:GLU:CG	2.81	0.59
1:A:49:PHE:CE1	1:A:53:CYS:SG	2.96	0.59
1:B:485:ARG:HB3	1:B:486:PRO:HD3	1.85	0.58
1:A:464:HIS:HE1	1:A:470:SER:H	1.50	0.58
1:B:50:ALA:O	1:B:54:VAL:HG23	2.03	0.58
1:A:283:LEU:O	1:A:286:LYS:N	2.36	0.58
1:B:23:VAL:O	1:B:27:PHE:HD1	1.87	0.58
1:A:571:GLU:N	1:A:571:GLU:OE1	2.36	0.58
1:B:36:PHE:O	1:B:40:VAL:HG23	2.04	0.57
1:A:30:TYR:OH	1:A:103:LEU:HD21	2.05	0.57
1:A:66:LEU:HB3	1:A:70:PHE:CE2	2.39	0.57
1:A:7:VAL:HG22	1:A:66:LEU:HD12	1.87	0.57
1:A:42:LEU:O	1:A:46:VAL:CG2	2.52	0.57
1:B:556:GLU:O	1:B:560:LYS:HG2	2.04	0.57
1:A:540:THR:HG21	1:A:544:LEU:HD11	1.81	0.56
1:A:141:GLU:O	1:A:145:ARG:HG3	2.05	0.56
1:A:222:ARG:CG	3:A:2017:HOH:O	2.36	0.56
1:A:186:ARG:O	1:A:190:LYS:HG3	2.05	0.56
1:A:178:LEU:O	1:A:179:LEU:C	2.43	0.56
1:A:29:GLN:HG2	1:A:147:PRO:HA	1.88	0.56
1:B:511:ALA:C	1:B:513:ILE:H	2.08	0.56
1:A:186:ARG:HD3	3:A:2010:HOH:O	2.05	0.55
1:B:464:HIS:HE1	1:B:470:SER:H	1.55	0.55
1:A:283:LEU:CG	1:A:284:LEU:N	2.68	0.55
1:A:199:LYS:HG2	1:A:211:PHE:HE2	1.72	0.55
1:B:120:VAL:HG21	1:B:175:ALA:CA	2.33	0.55
1:A:30:TYR:OH	1:A:103:LEU:CD2	2.55	0.55
1:A:472:ARG:NH1	1:A:494:ASP:HB2	2.22	0.55
1:B:475:LYS:O	1:B:479:GLU:HB2	2.05	0.55
1:A:502:PHE:CD1	2:A:4002:PFL:H113	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:TYR:HE1	3:A:2060:HOH:O	1.88	0.54
1:A:564:LYS:C	1:A:566:THR:H	2.09	0.54
1:B:115:LEU:HD22	1:B:145:ARG:NH1	2.22	0.54
1:B:566:THR:O	1:B:570:GLU:N	2.40	0.54
1:A:366:PRO:C	1:A:368:GLU:N	2.60	0.54
1:A:563:ASP:CG	1:A:564:LYS:O	2.46	0.54
1:B:240:LYS:HE2	1:B:244:GLU:OE2	2.07	0.54
1:A:511:ALA:O	1:A:513:ILE:N	2.41	0.53
1:A:540:THR:HG23	1:A:544:LEU:HG	1.90	0.53
1:B:325:VAL:HG12	1:B:329:MET:CE	2.38	0.53
1:A:532:LEU:HG	2:A:4002:PFL:C8	2.38	0.53
1:A:485:ARG:CZ	1:A:486:PRO:HD3	2.38	0.53
1:B:103:LEU:O	1:B:105:HIS:N	2.41	0.53
1:B:464:HIS:CE1	1:B:470:SER:H	2.26	0.53
1:B:19:PHE:CE1	1:B:47:THR:HG23	2.44	0.53
1:A:283:LEU:HG	1:A:284:LEU:H	1.72	0.53
1:A:81:ARG:CB	1:A:85:GLY:HA2	2.39	0.53
1:A:373:VAL:HG13	1:A:374:PHE:N	2.24	0.53
1:A:218:ARG:NH2	3:A:2017:HOH:O	2.40	0.53
1:A:508:THR:CG2	1:A:510:HIS:CE1	2.92	0.53
1:A:66:LEU:HD21	3:A:2001:HOH:O	2.08	0.53
1:A:49:PHE:HE1	1:A:62:CYS:SG	2.31	0.52
1:B:483:ASN:C	1:B:486:PRO:HD2	2.29	0.52
1:A:178:LEU:HG	1:A:182:LEU:HG	1.91	0.52
1:A:366:PRO:C	1:A:368:GLU:H	2.12	0.52
1:B:19:PHE:C	1:B:19:PHE:CD1	2.82	0.52
1:B:212:LYS:O	1:B:216:VAL:HG23	2.08	0.52
1:A:98:ARG:NH1	1:A:99:ASN:HB2	2.24	0.52
1:A:110:PRO:HB2	1:A:112:LEU:HG	1.90	0.52
1:A:405:ASN:O	1:A:409:VAL:HG23	2.10	0.52
1:A:485:ARG:NH2	1:A:486:PRO:HG3	2.25	0.52
1:A:27:PHE:CE2	1:A:74:LEU:HG	2.45	0.52
1:A:117:ARG:HB2	1:A:123:MET:CE	2.40	0.52
1:B:30:TYR:HE1	1:B:103:LEU:HD23	1.75	0.52
1:A:472:ARG:HH11	1:A:494:ASP:HB2	1.75	0.52
1:A:43:VAL:O	1:A:47:THR:OG1	2.27	0.52
1:B:410:ARG:NE	3:B:2040:HOH:O	2.43	0.51
1:A:311:GLU:O	1:A:367:HIS:HE1	1.94	0.51
1:A:325:VAL:HG12	1:A:329:MET:HE2	1.91	0.51
1:A:464:HIS:CE1	1:A:470:SER:H	2.28	0.51
1:B:81:ARG:HG2	1:B:88:ALA:CB	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:GLU:HB3	1:A:384:PRO:HD3	1.92	0.51
1:B:370:TYR:C	1:B:370:TYR:CD1	2.84	0.51
1:B:54:VAL:HG12	1:B:55:ALA:N	2.25	0.51
1:B:178:LEU:HG	1:B:182:LEU:HG	1.91	0.51
1:B:541:LYS:H	1:B:543:GLN:HG3	1.75	0.51
1:A:67:HIS:CG	1:A:98:ARG:HH21	2.29	0.50
1:B:87:MET:HE1	1:B:105:HIS:HB3	1.93	0.50
2:A:4001:PFL:H111	3:A:2036:HOH:O	2.11	0.50
1:A:563:ASP:C	1:A:564:LYS:O	2.42	0.50
1:B:531:GLU:O	1:B:535:HIS:CD2	2.63	0.50
1:B:394:LEU:HD11	1:B:398:LEU:HD11	1.94	0.50
1:B:31:LEU:HB3	1:B:34:CYS:HB2	1.94	0.50
1:A:30:TYR:CE1	1:A:103:LEU:HD23	2.46	0.50
1:A:168:CYS:SG	1:A:177:CYS:C	2.90	0.50
1:A:325:VAL:HG12	1:A:329:MET:CE	2.42	0.50
1:A:381:VAL:O	1:A:384:PRO:HD2	2.12	0.50
1:B:139:LEU:HD21	1:B:158:ALA:HB2	1.94	0.50
1:B:420:THR:HB	1:B:421:PRO:HD3	1.94	0.50
1:B:57:GLU:OE1	1:B:57:GLU:HA	2.10	0.50
1:A:32:GLN:NE2	1:A:110:PRO:HG3	2.27	0.50
1:A:61:ASN:O	1:A:63:ASP:N	2.45	0.50
1:A:139:LEU:HD21	1:A:158:ALA:HB2	1.94	0.49
1:A:97:GLU:O	1:A:98:ARG:C	2.49	0.49
1:A:212:LYS:O	1:A:216:VAL:HG23	2.11	0.49
1:A:240:LYS:HE2	1:A:244:GLU:OE2	2.13	0.49
1:A:34:CYS:HB3	1:A:39:HIS:HE2	1.78	0.49
1:A:420:THR:HB	1:A:421:PRO:HD3	1.94	0.49
1:B:206:PHE:CE2	1:B:481:LEU:HD13	2.47	0.49
1:A:198:LEU:HA	1:A:458:ASN:ND2	2.28	0.49
1:A:420:THR:HG23	1:A:530:VAL:CG1	2.43	0.49
1:B:373:VAL:HG13	1:B:374:PHE:HD1	1.78	0.49
1:B:61:ASN:HB3	1:B:64:LYS:HE2	1.94	0.49
1:A:511:ALA:CB	1:A:565:GLU:HG3	2.43	0.49
1:A:564:LYS:C	1:A:566:THR:N	2.66	0.49
1:B:16:GLU:O	1:B:20:LYS:HG2	2.12	0.49
1:A:356:THR:O	1:A:360:CYS:HB2	2.12	0.49
1:B:405:ASN:O	1:B:409:VAL:HG23	2.13	0.49
1:B:520:GLU:HG3	3:B:2060:HOH:O	2.11	0.49
1:B:542:GLU:O	1:B:545:LYS:HG3	2.12	0.49
1:A:87:MET:HE3	1:A:105:HIS:HB3	1.95	0.49
1:B:9:HIS:NE2	1:B:13:ASP:OD2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:GLN:NE2	3:B:2014:HOH:O	2.45	0.49
1:B:198:LEU:HA	1:B:458:ASN:ND2	2.28	0.49
1:A:370:TYR:CD1	1:A:370:TYR:C	2.87	0.48
1:A:529:LEU:O	1:A:533:VAL:HG23	2.13	0.48
1:B:398:LEU:O	1:B:402:LYS:HB2	2.12	0.48
1:A:232:SER:O	1:A:236:THR:OG1	2.31	0.48
1:B:135:LEU:HD11	1:B:162:LYS:HB2	1.95	0.48
1:A:23:VAL:O	1:A:27:PHE:HD1	1.97	0.48
1:B:442:GLU:HA	1:B:445:ARG:HD2	1.95	0.48
1:A:153:GLU:HG2	1:A:257:ARG:HH12	1.78	0.48
1:A:117:ARG:HB2	1:A:123:MET:HE1	1.95	0.48
1:B:511:ALA:C	1:B:513:ILE:N	2.66	0.48
1:A:464:HIS:HE1	1:A:469:VAL:H	1.62	0.48
1:A:49:PHE:CD1	1:A:49:PHE:C	2.87	0.48
1:B:23:VAL:O	1:B:27:PHE:CD1	2.67	0.48
1:B:38:ASP:O	1:B:41:LYS:HB3	2.13	0.48
1:B:571:GLU:HA	1:B:574:LYS:HB2	1.96	0.48
1:A:66:LEU:O	1:A:70:PHE:CD2	2.64	0.48
1:A:512:ASP:O	1:A:515:THR:HG22	2.14	0.47
1:B:381:VAL:O	1:B:384:PRO:HD2	2.14	0.47
1:B:579:SER:HB2	2:B:4002:PFL:HC7	1.95	0.47
1:A:49:PHE:HE1	1:A:53:CYS:SG	2.37	0.47
1:B:100:GLU:O	1:B:104:GLN:CG	2.61	0.47
1:B:75:CYS:HA	1:B:78:ALA:HB3	1.97	0.47
1:B:95:GLU:OE1	1:B:95:GLU:HA	2.13	0.47
1:A:127:PHE:CE1	1:A:131:GLU:HG3	2.49	0.47
1:A:38:ASP:OD1	1:A:38:ASP:N	2.46	0.47
1:A:64:LYS:HB2	1:A:69:LEU:HD21	1.96	0.47
1:B:516:LEU:HD22	1:B:520:GLU:OE1	2.14	0.47
1:A:30:TYR:HE1	1:A:103:LEU:HD23	1.79	0.47
1:A:508:THR:CG2	1:A:510:HIS:ND1	2.77	0.47
1:A:279:CYS:HA	1:A:286:LYS:CD	2.42	0.47
1:A:98:ARG:NH1	1:A:99:ASN:CB	2.78	0.47
1:B:366:PRO:O	1:B:369:CYS:N	2.47	0.47
1:A:224:PRO:HB2	1:A:299:PRO:HD3	1.97	0.47
1:A:6:GLU:C	1:A:8:ALA:N	2.68	0.47
1:B:118:PRO:HB2	1:B:122:VAL:HB	1.97	0.47
1:A:90:CYS:HA	1:A:93:LYS:HG3	1.97	0.47
1:B:14:LEU:HD13	1:B:22:LEU:HD12	1.96	0.47
1:A:61:ASN:C	1:A:63:ASP:N	2.69	0.47
1:B:540:THR:HB	1:B:544:LEU:HG	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:SER:HB2	1:A:57:GLU:HG2	1.98	0.46
1:A:223:PHE:CD1	1:A:272:SER:HB2	2.51	0.46
1:A:513:ILE:HA	1:A:516:LEU:HD12	1.96	0.46
1:A:156:PHE:HE1	1:A:285:GLU:HG3	1.80	0.46
1:A:179:LEU:CB	1:A:180:PRO:CD	2.94	0.46
1:B:464:HIS:CE1	1:B:469:VAL:H	2.34	0.46
1:A:420:THR:HG23	1:A:530:VAL:HG11	1.96	0.46
1:A:66:LEU:HB3	1:A:70:PHE:HE2	1.78	0.46
1:B:290:ILE:O	1:B:293:VAL:HG12	2.15	0.46
1:A:410:ARG:CD	3:A:2035:HOH:O	1.97	0.46
1:A:49:PHE:O	1:A:49:PHE:HD1	1.98	0.46
1:A:97:GLU:HA	1:A:98:ARG:HH12	1.79	0.46
1:B:5:SER:HA	1:B:62:CYS:O	2.15	0.46
1:B:9:HIS:CD2	1:B:13:ASP:OD2	2.69	0.46
1:A:81:ARG:CA	1:A:85:GLY:HA2	2.46	0.46
1:A:67:HIS:CB	1:A:98:ARG:HH21	2.27	0.46
1:B:344:VAL:HG12	1:B:482:VAL:HG13	1.97	0.46
1:B:279:CYS:HA	1:B:286:LYS:CD	2.45	0.46
1:A:224:PRO:HD2	1:A:296:ASP:HB3	1.97	0.46
1:A:572:GLY:O	1:A:576:VAL:HG23	2.15	0.46
1:A:306:ALA:CA	1:A:310:VAL:HG22	2.41	0.45
1:A:93:LYS:HB2	1:A:98:ARG:HA	1.98	0.45
1:B:556:GLU:CG	1:B:557:LYS:H	2.25	0.45
1:A:520:GLU:HA	1:A:523:ILE:HD12	1.98	0.45
1:A:173:ASP:HB3	1:A:176:ALA:HB3	1.98	0.45
1:A:99:ASN:O	1:A:100:GLU:C	2.54	0.45
1:B:510:HIS:CB	1:B:512:ASP:OD1	2.65	0.45
1:B:57:GLU:HB3	1:B:58:SER:H	1.57	0.45
1:A:196:GLN:HE22	1:A:242:HIS:CE1	2.35	0.45
1:A:551:PHE:O	1:A:555:VAL:HG23	2.17	0.45
1:B:194:ALA:HB1	1:B:455:VAL:CG1	2.47	0.45
1:A:98:ARG:NH2	1:A:99:ASN:HB2	2.30	0.45
1:B:364:ALA:O	1:B:366:PRO:HD3	2.17	0.45
1:A:378:LYS:HB3	1:A:379:PRO:CD	2.42	0.45
1:A:7:VAL:CG2	1:A:66:LEU:HD12	2.47	0.45
1:A:6:GLU:O	1:A:8:ALA:N	2.49	0.45
1:B:393:GLU:HA	1:B:396:GLU:HG3	1.98	0.45
1:A:280:GLU:HA	1:A:280:GLU:OE1	2.17	0.44
1:B:570:GLU:O	1:B:574:LYS:HE3	2.17	0.44
1:A:49:PHE:HD1	1:A:49:PHE:C	2.20	0.44
1:A:66:LEU:CD1	1:A:66:LEU:N	2.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:SER:HB2	1:A:421:PRO:HD2	1.98	0.44
1:B:333:GLU:OE1	1:B:336:ARG:HD3	2.17	0.44
1:B:372:LYS:O	1:B:375:ASP:HB2	2.16	0.44
1:B:34:CYS:HB3	1:B:39:HIS:CD2	2.51	0.44
1:B:551:PHE:O	1:B:555:VAL:HG23	2.16	0.44
1:A:109:ASN:HA	1:A:109:ASN:HD22	1.68	0.44
1:A:95:GLU:O	1:A:96:PRO:C	2.53	0.44
1:B:441:PRO:C	1:B:443:ALA:N	2.70	0.44
1:A:522:GLN:CA	3:A:2060:HOH:O	2.65	0.44
1:A:137:LYS:O	1:A:141:GLU:HG2	2.17	0.44
1:A:433:VAL:HG22	1:A:452:TYR:HE2	1.80	0.44
1:B:367:HIS:CE1	3:B:2031:HOH:O	2.71	0.44
1:B:516:LEU:HD22	1:B:520:GLU:HB3	1.98	0.44
1:A:360:CYS:SG	1:A:370:TYR:N	2.91	0.44
1:A:38:ASP:O	1:A:42:LEU:HG	2.17	0.44
1:B:51:LYS:C	1:B:53:CYS:H	2.21	0.44
1:A:78:ALA:C	1:A:80:LEU:H	2.21	0.43
1:B:555:VAL:O	1:B:556:GLU:C	2.56	0.43
1:A:179:LEU:CB	1:A:180:PRO:HD3	2.48	0.43
1:A:274:LYS:HE3	1:A:296:ASP:HA	1.99	0.43
1:A:61:ASN:C	1:A:63:ASP:H	2.20	0.43
1:A:274:LYS:HE2	1:A:297:GLU:OE1	2.18	0.43
1:B:397:GLN:HG3	1:B:398:LEU:CD2	2.48	0.43
1:A:283:LEU:HD12	1:A:283:LEU:C	2.39	0.43
1:B:283:LEU:CG	1:B:284:LEU:N	2.82	0.43
1:A:196:GLN:HE22	1:A:242:HIS:HE1	1.67	0.43
1:A:114:ARG:HA	3:A:2005:HOH:O	2.19	0.43
1:A:503:ASN:ND2	1:A:505:GLU:N	2.67	0.43
1:A:508:THR:HG23	1:A:510:HIS:ND1	2.34	0.43
1:A:566:THR:O	1:A:569:ALA:N	2.49	0.43
1:B:64:LYS:HE2	1:B:69:LEU:HD23	2.00	0.43
1:A:115:LEU:HD22	1:A:145:ARG:NH1	2.33	0.43
1:A:434:GLY:O	1:A:438:CYS:HB2	2.18	0.43
1:B:272:SER:HB3	1:B:275:LEU:HG	2.01	0.43
1:B:57:GLU:O	1:B:59:ALA:N	2.52	0.43
1:A:543:GLN:HG2	1:A:543:GLN:H	1.47	0.43
1:A:277:GLU:O	1:A:277:GLU:HG2	2.19	0.43
1:A:485:ARG:CB	1:A:486:PRO:CD	2.81	0.43
1:A:503:ASN:HD21	1:A:505:GLU:HB2	1.83	0.43
1:B:109:ASN:HB3	1:B:466:LYS:NZ	2.34	0.43
1:B:408:LEU:HD11	1:B:526:GLN:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:LYS:C	1:A:542:GLU:HG3	2.40	0.42
1:B:342:SER:OG	1:B:344:VAL:HG23	2.19	0.42
1:B:117:ARG:HA	1:B:118:PRO:HD3	1.86	0.42
1:B:17:GLU:HA	1:B:20:LYS:HE2	2.01	0.42
1:B:21:ALA:O	1:B:25:ILE:HG13	2.18	0.42
1:B:103:LEU:C	1:B:105:HIS:H	2.22	0.42
1:B:168:CYS:SG	1:B:177:CYS:C	2.98	0.42
1:B:185:LEU:HD23	1:B:185:LEU:HA	1.90	0.42
1:B:37:GLU:CD	1:B:37:GLU:H	2.23	0.42
1:B:572:GLY:O	1:B:576:VAL:HG23	2.20	0.42
1:B:70:PHE:CD1	1:B:70:PHE:N	2.88	0.42
1:A:319:TYR:CE1	1:A:323:LYS:HB2	2.54	0.42
1:B:98:ARG:O	1:B:101:CYS:HB3	2.20	0.42
1:B:22:LEU:HD21	1:B:155:LEU:HD11	2.01	0.42
1:B:178:LEU:O	1:B:179:LEU:C	2.58	0.42
1:A:366:PRO:O	1:A:367:HIS:C	2.57	0.42
1:A:5:SER:CB	1:A:57:GLU:HG2	2.50	0.42
1:A:99:ASN:C	1:A:101:CYS:N	2.69	0.42
1:B:141:GLU:HA	1:B:141:GLU:OE1	2.20	0.42
1:A:531:GLU:O	1:A:535:HIS:CD2	2.73	0.42
1:B:137:LYS:O	1:B:141:GLU:HG2	2.19	0.42
1:B:94:GLN:O	1:B:97:GLU:HB2	2.20	0.42
1:A:231:VAL:O	1:A:235:VAL:HG23	2.20	0.41
1:A:493:VAL:HG22	1:A:493:VAL:O	2.20	0.41
1:A:214:TRP:CD1	1:A:343:VAL:HG11	2.55	0.41
1:A:283:LEU:O	1:A:284:LEU:C	2.59	0.41
1:A:410:ARG:NH2	2:A:4001:PFL:C12	2.83	0.41
1:B:532:LEU:HA	1:B:532:LEU:HD23	1.87	0.41
1:A:247:HIS:O	1:A:247:HIS:CD2	2.73	0.41
1:B:522:GLN:HA	1:B:525:LYS:HB2	2.02	0.41
1:B:85:GLY:C	1:B:87:MET:H	2.24	0.41
1:A:566:THR:C	1:A:568:PHE:N	2.70	0.41
1:A:452:TYR:O	1:A:456:VAL:HG23	2.21	0.41
1:B:367:HIS:HA	1:B:370:TYR:CZ	2.56	0.41
1:B:567:CYS:O	1:B:571:GLU:HB2	2.20	0.41
1:A:415:VAL:HG23	1:A:415:VAL:O	2.21	0.41
1:A:41:LYS:O	1:A:45:GLU:HG3	2.21	0.41
1:A:511:ALA:CB	1:A:565:GLU:CB	2.97	0.41
1:A:7:VAL:HG21	1:A:69:LEU:HD13	2.03	0.41
1:B:278:CYS:HB3	1:B:289:CYS:HB3	1.95	0.41
1:A:333:GLU:OE1	1:A:336:ARG:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:GLU:HA	1:A:17:GLU:OE1	2.21	0.41
1:A:16:GLU:O	1:A:20:LYS:HB2	2.21	0.41
1:A:302:LEU:HA	1:A:302:LEU:HD23	1.95	0.41
1:A:37:GLU:CD	1:A:37:GLU:H	2.23	0.41
1:A:538:LYS:O	1:A:539:ALA:C	2.59	0.41
1:B:249:ASP:CB	1:B:252:GLU:OE1	2.59	0.41
1:B:373:VAL:HG13	1:B:374:PHE:N	2.35	0.41
1:B:64:LYS:HE2	1:B:69:LEU:CD2	2.51	0.41
1:A:67:HIS:CE1	1:A:99:ASN:ND2	2.89	0.41
1:A:222:ARG:C	1:A:224:PRO:HD3	2.41	0.40
1:A:247:HIS:O	1:A:247:HIS:CG	2.74	0.40
1:A:514:CYS:HA	1:A:521:ARG:HH21	1.85	0.40
1:A:398:LEU:HG	1:A:398:LEU:H	1.75	0.40
1:A:563:ASP:O	1:A:564:LYS:C	2.59	0.40
1:B:113:PRO:O	1:B:145:ARG:NH2	2.54	0.40
1:B:179:LEU:HB2	1:B:180:PRO:HD3	2.03	0.40
1:A:503:ASN:C	1:A:503:ASN:ND2	2.75	0.40
1:B:567:CYS:O	1:B:571:GLU:N	2.35	0.40
1:A:272:SER:HB3	1:A:275:LEU:HG	2.03	0.40
1:B:153:GLU:O	1:B:157:PHE:HD1	2.02	0.40
1:B:556:GLU:CG	1:B:557:LYS:N	2.76	0.40
1:A:123:MET:HB3	1:A:165:PHE:CE2	2.56	0.40
1:A:407:LEU:HD21	2:A:4001:PFL:H123	2.02	0.40
1:B:32:GLN:HE21	1:B:110:PRO:HG3	1.85	0.40
1:B:282:PRO:HB2	1:B:285:GLU:OE1	2.21	0.40
1:B:333:GLU:O	1:B:337:ARG:HG3	2.20	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	576/585 (98%)	503 (87%)	59 (10%)	14 (2%)	6	3
1	B	576/585 (98%)	513 (89%)	49 (8%)	14 (2%)	6	3
All	All	1152/1170 (98%)	1016 (88%)	108 (9%)	28 (2%)	6	3

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	ALA
1	A	98	ARG
1	A	300	ALA
1	A	366	PRO
1	A	367	HIS
1	A	510	HIS
1	A	538	LYS
1	B	54	VAL
1	B	57	GLU
1	B	58	SER
1	B	60	GLU
1	A	62	CYS
1	A	512	ASP
1	B	85	GLY
1	B	104	GLN
1	B	300	ALA
1	B	555	VAL
1	A	97	GLU
1	B	537	PRO
1	B	565	GLU
1	A	179	LEU
1	A	180	PRO
1	A	283	LEU
1	B	77	VAL
1	B	86	GLU
1	B	75	CYS
1	A	537	PRO
1	B	179	LEU

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	474/511 (93%)	419 (88%)	55 (12%)	5	5
1	B	475/511 (93%)	424 (89%)	51 (11%)	6	6
All	All	949/1022 (93%)	843 (89%)	106 (11%)	6	5

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	TYR
1	A	37	GLU
1	A	38	ASP
1	A	47	THR
1	A	49	PHE
1	A	64	LYS
1	A	66	LEU
1	A	72	ASP
1	A	79	THR
1	A	83	THR
1	A	86	GLU
1	A	87	MET
1	A	98	ARG
1	A	109	ASN
1	A	124	CYS
1	A	144	ARG
1	A	174	LYS
1	A	179	LEU
1	A	195	LYS
1	A	212	LYS
1	A	232	SER
1	A	233	LYS
1	A	236	THR
1	A	245	CYS
1	A	249	ASP
1	A	276	LYS
1	A	281	LYS
1	A	283	LEU
1	A	284	LEU
1	A	287	SER
1	A	301	ASP
1	A	317	LYS
1	A	323	LYS

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Mol	Chain	Res	Type
1	A	334	TYR
1	A	336	ARG
1	A	337	ARG
1	A	370	TYR
1	A	375	ASP
1	A	398	LEU
1	A	414	LYS
1	A	435	SER
1	A	441	PRO
1	A	445	ARG
1	A	467	THR
1	A	471	ASP
1	A	486	PRO
1	A	500	LYS
1	A	503	ASN
1	A	508	THR
1	A	512	ASP
1	A	513	ILE
1	A	532	LEU
1	A	543	GLN
1	A	550	ASP
1	A	568	PHE
1	B	19	PHE
1	B	33	GLN
1	B	34	CYS
1	B	38	ASP
1	B	56	ASP
1	B	57	GLU
1	B	58	SER
1	B	64	LYS
1	B	79	THR
1	B	82	GLU
1	B	83	THR
1	B	105	HIS
1	B	174	LYS
1	B	179	LEU
1	B	204	GLN
1	B	209	ARG
1	B	212	LYS
1	B	232	SER
1	B	233	LYS
1	B	276	LYS

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Mol	Chain	Res	Type
1	B	280	GLU
1	B	281	LYS
1	B	283	LEU
1	B	284	LEU
1	B	292	GLU
1	B	305	LEU
1	B	314	ASP
1	B	323	LYS
1	B	324	ASP
1	B	336	ARG
1	B	337	ARG
1	B	344	VAL
1	B	370	TYR
1	B	375	ASP
1	B	392	CYS
1	B	398	LEU
1	B	414	LYS
1	B	435	SER
1	B	467	THR
1	B	480	SER
1	B	489	SER
1	B	499	PRO
1	B	519	LYS
1	B	524	LYS
1	B	532	LEU
1	B	540	THR
1	B	543	GLN
1	B	550	ASP
1	B	564	LYS
1	B	566	THR
1	B	568	PHE

Some 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	130	ASN
1	A	196	GLN
1	A	247	HIS
1	A	367	HIS

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Mol	Chain	Res	Type
1	A	385	GLN
1	A	464	HIS
1	A	483	ASN
1	A	503	ASN
1	A	535	HIS
1	A	543	GLN
1	B	33	GLN
1	B	196	GLN
1	B	385	GLN
1	B	464	HIS
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](#)

4 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	PFL	B	4002	-	13,13,13	1.44	4 (30%)	18,18,18	1.01	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PFL	A	4001	-	13,13,13	1.76	5 (38%)	18,18,18	0.82	0
2	PFL	A	4002	-	13,13,13	1.60	3 (23%)	18,18,18	0.96	1 (5%)
2	PFL	B	4001	-	13,13,13	1.75	5 (38%)	18,18,18	0.84	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	PFL	B	4002	-	-	0/8/8/8	0/1/1/1
2	PFL	A	4001	-	-	0/8/8/8	0/1/1/1
2	PFL	A	4002	-	-	0/8/8/8	0/1/1/1
2	PFL	B	4001	-	-	0/8/8/8	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4001	PFL	C5-C6	3.12	1.43	1.39
2	B	4001	PFL	C5-C6	3.05	1.43	1.39
2	A	4002	PFL	C5-C6	2.96	1.43	1.39
2	B	4001	PFL	C1-C2	2.86	1.44	1.39
2	A	4001	PFL	C1-C2	2.82	1.44	1.39
2	B	4002	PFL	C1-C2	2.66	1.43	1.39
2	B	4002	PFL	C5-C6	2.49	1.43	1.39
2	B	4001	PFL	C3-C2	2.47	1.43	1.39
2	A	4001	PFL	C3-C2	2.42	1.42	1.39
2	A	4002	PFL	C3-C2	2.40	1.42	1.39
2	A	4002	PFL	C6-C10	2.34	1.55	1.52
2	B	4002	PFL	C6-C10	2.24	1.55	1.52
2	B	4001	PFL	O1-C1	2.18	1.42	1.37
2	A	4001	PFL	O1-C1	2.15	1.42	1.37
2	B	4002	PFL	C3-C2	2.10	1.42	1.39
2	A	4001	PFL	C6-C10	2.03	1.55	1.52
2	B	4001	PFL	C6-C10	2.00	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4002	PFL	C3-C2-C7	2.17	123.08	119.92

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	4002	PFL	5	0
2	A	4001	PFL	4	0
2	A	4002	PFL	3	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%)	0.74	68 (11%) 4 4	18, 54, 105, 121	0
1	B	578/585 (98%)	0.82	90 (15%) 2 1	22, 57, 113, 129	0
All	All	1156/1170 (98%)	0.78	158 (13%) 3 2	18, 56, 110, 129	0

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	539	ALA	10.9
1	A	85	GLY	8.3
1	B	87	MET	8.0
1	B	83	THR	7.8
1	B	561	ALA	7.0
1	A	178	LEU	6.9
1	A	83	THR	6.8
1	A	91	CYS	6.6
1	A	87	MET	6.5
1	A	96	PRO	6.4
1	B	78	ALA	6.2
1	B	539	ALA	5.9
1	A	79	THR	5.7
1	B	90	CYS	5.5
1	B	91	CYS	5.3
1	B	164	ALA	5.3
1	A	165	PHE	5.2
1	B	568	PHE	5.1
1	B	102	PHE	5.1
1	B	79	THR	5.0
1	B	174	LYS	5.0
1	B	513	ILE	4.8
1	B	80	LEU	4.8
1	B	84	TYR	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	276	LYS	4.7
1	B	120	VAL	4.6
1	A	174	LYS	4.5
1	B	566	THR	4.5
1	B	94	GLN	4.5
1	A	84	TYR	4.5
1	B	98	ARG	4.4
1	A	560	LYS	4.4
1	A	164	ALA	4.4
1	B	540	THR	4.3
1	A	169	CYS	4.2
1	B	567	CYS	4.1
1	A	55	ALA	4.1
1	A	563	ASP	4.1
1	A	557	LYS	4.1
1	B	564	LYS	4.0
1	B	123	MET	4.0
1	B	562	ASP	4.0
1	A	78	ALA	4.0
1	B	54	VAL	4.0
1	A	513	ILE	3.9
1	A	168	CYS	3.9
1	A	567	CYS	3.9
1	B	563	ASP	3.9
1	B	85	GLY	3.9
1	A	561	ALA	3.8
1	A	95	GLU	3.8
1	B	93	LYS	3.8
1	A	88	ALA	3.8
1	A	511	ALA	3.7
1	A	123	MET	3.7
1	B	5	SER	3.7
1	A	568	PHE	3.7
1	B	175	ALA	3.6
1	A	554	PHE	3.6
1	A	90	CYS	3.5
1	A	80	LEU	3.5
1	B	179	LEU	3.5
1	B	178	LEU	3.4
1	B	55	ALA	3.4
1	B	86	GLU	3.4
1	B	300	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	57	GLU	3.3
1	A	182	LEU	3.3
1	B	572	GLY	3.3
1	A	179	LEU	3.2
1	B	582	ALA	3.2
1	A	540	THR	3.2
1	A	171	ALA	3.1
1	A	276	LYS	3.1
1	B	77	VAL	3.1
1	A	570	GLU	3.1
1	A	49	PHE	3.1
1	A	94	GLN	3.0
1	B	88	ALA	3.0
1	B	516	LEU	3.0
1	B	82	GLU	3.0
1	A	81	ARG	3.0
1	A	578	ALA	3.0
1	A	7	VAL	2.9
1	B	519	LYS	2.9
1	A	572	GLY	2.9
1	A	57	GLU	2.9
1	B	115	LEU	2.8
1	B	510	HIS	2.8
1	A	516	LEU	2.8
1	B	557	LYS	2.8
1	A	556	GLU	2.8
1	B	560	LYS	2.8
1	B	466	LYS	2.7
1	B	81	ARG	2.7
1	A	98	ARG	2.7
1	B	558	CYS	2.7
1	B	21	ALA	2.7
1	B	30	TYR	2.7
1	B	52	THR	2.7
1	B	577	ALA	2.6
1	B	515	THR	2.6
1	B	565	GLU	2.6
1	B	364	ALA	2.6
1	B	511	ALA	2.6
1	B	56	ASP	2.5
1	A	54	VAL	2.5
1	A	56	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	63	ASP	2.5
1	B	275	LEU	2.5
1	A	64	LYS	2.5
1	A	120	VAL	2.4
1	B	31	LEU	2.4
1	A	247	HIS	2.4
1	B	555	VAL	2.4
1	A	310	VAL	2.4
1	B	89	ASP	2.4
1	B	97	GLU	2.4
1	B	74	LEU	2.4
1	A	176	ALA	2.4
1	A	562	ASP	2.4
1	A	280	GLU	2.4
1	B	33	GLN	2.4
1	B	116	VAL	2.4
1	A	573	LYS	2.3
1	B	574	LYS	2.3
1	B	75	CYS	2.3
1	B	397	GLN	2.3
1	A	8	ALA	2.3
1	B	166	THR	2.3
1	A	102	PHE	2.3
1	B	165	PHE	2.3
1	A	31	LEU	2.3
1	B	171	ALA	2.3
1	B	182	LEU	2.2
1	B	7	VAL	2.2
1	B	559	CYS	2.2
1	B	247	HIS	2.2
1	B	12	LYS	2.2
1	B	547	VAL	2.2
1	A	509	PHE	2.2
1	B	95	GLU	2.2
1	A	564	LYS	2.2
1	A	273	SER	2.2
1	B	514	CYS	2.2
1	B	279	CYS	2.1
1	A	5	SER	2.1
1	B	181	LYS	2.1
1	A	571	GLU	2.1
1	B	49	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	92	ALA	2.1
1	A	367	HIS	2.0
1	B	62	CYS	2.0
1	B	169	CYS	2.0
1	A	69	LEU	2.0
1	B	92	ALA	2.0
1	A	93	LYS	2.0
1	B	177	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. 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(\AA^2)	Q<0.9
2	PFL	B	4001	13/13	0.78	0.36	65,68,71,72	0
2	PFL	B	4002	13/13	0.79	0.31	87,88,89,90	0
2	PFL	A	4001	13/13	0.83	0.32	60,62,66,67	0
2	PFL	A	4002	13/13	0.87	0.22	76,77,79,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.