



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:35 AM UTC

PDB ID : 1E7A / pdb_00001e7a
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 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

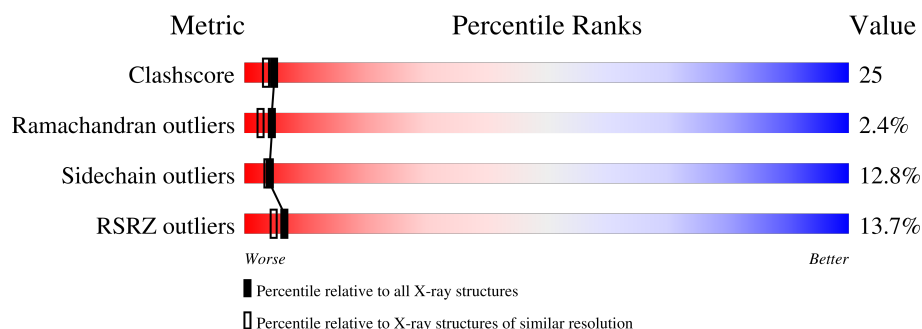
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 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	

2 Entry composition [i](#)

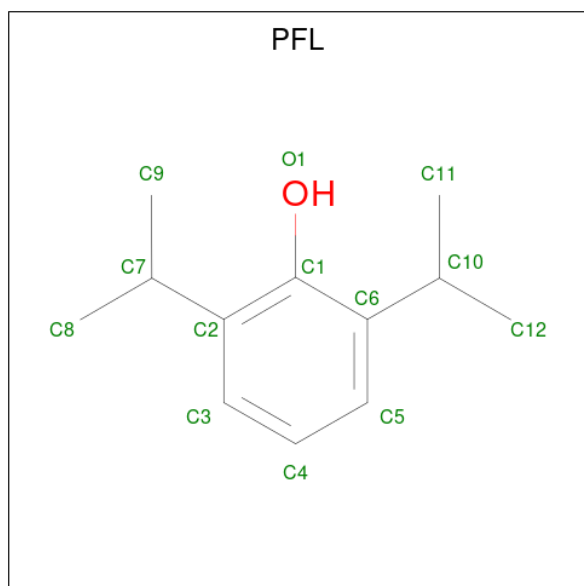
There are 3 unique types of molecules in this entry. The entry contains 9122 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: PFL) (formula: C₁₂H₁₈O).



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		

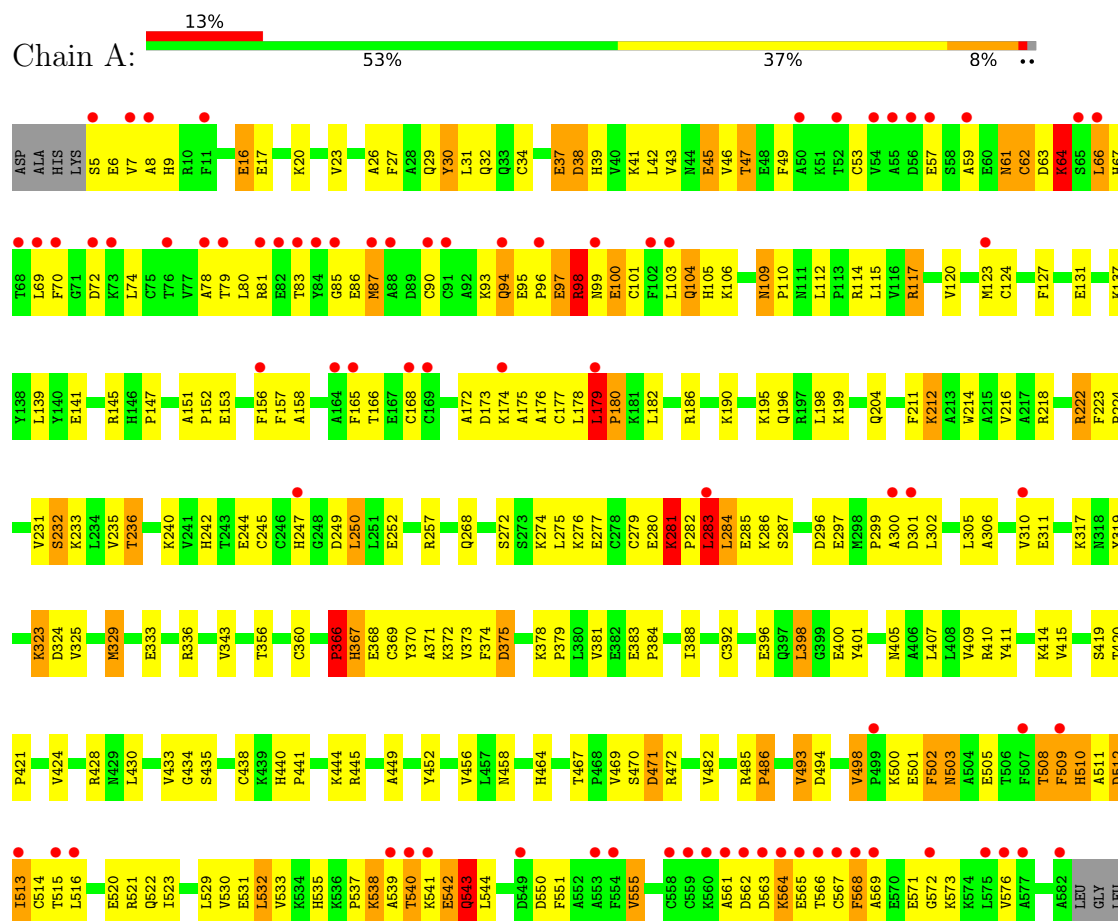
- Molecule 3 is water.

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

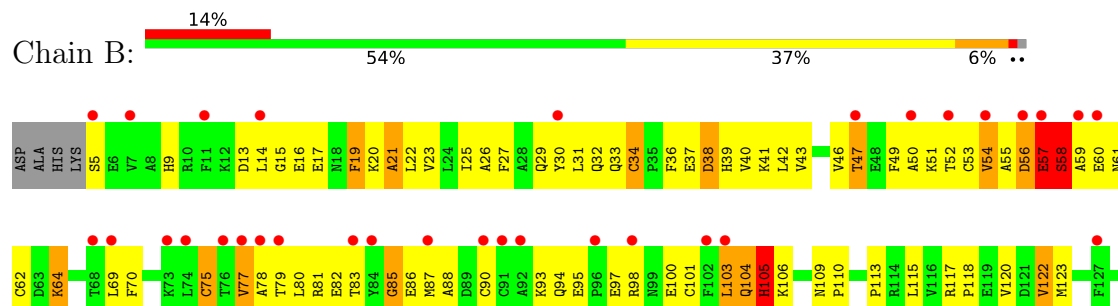
3 Residue-property plots

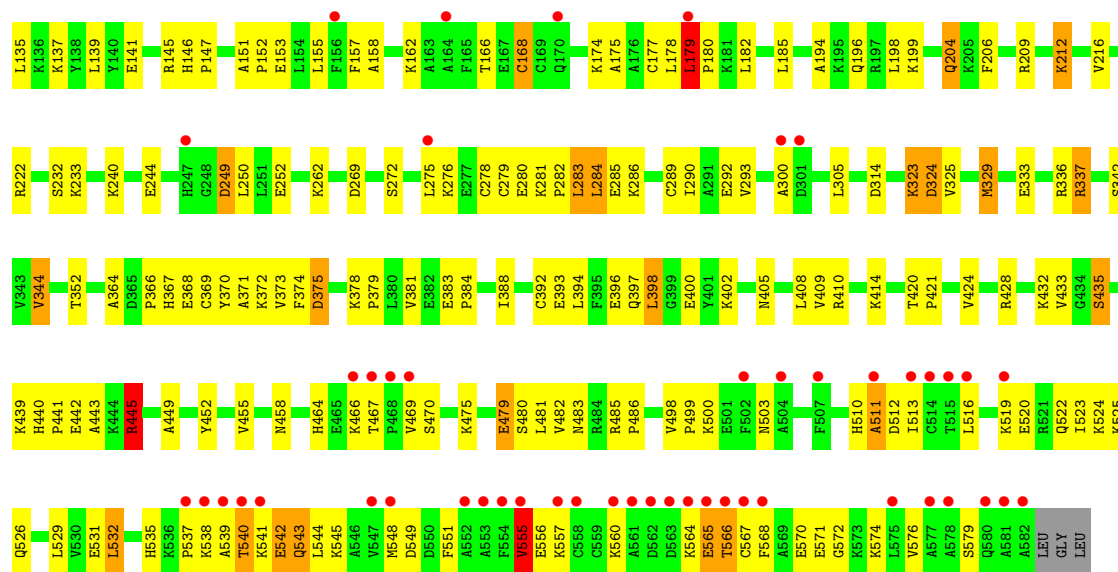
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	55.40Å 55.61Å 120.50Å 81.11° 90.57° 65.50°	Depositor
Resolution (Å)	30.00 – 2.20 30.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.1 (30.00-2.20) 96.1 (30.00-2.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 2.20Å)	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)	0.36 , 82.7	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 ⓘ

5.1 Standard geometry ⓘ

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	0.53	3/4558 (0.1%)	1.04	26/6174 (0.4%)
1	B	0.43	2/4565 (0.0%)	0.91	21/6178 (0.3%)
All	All	0.49	5/9123 (0.1%)	0.98	47/12352 (0.4%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	502	PHE	N-CA	-6.99	1.37	1.46
1	A	501	GLU	CA-C	-6.19	1.45	1.52
1	B	105	HIS	N-CA	5.50	1.51	1.46
1	B	500	LYS	N-CA	-5.42	1.39	1.45
1	A	542	GLU	N-CA	-5.39	1.41	1.46

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	543	GLN	N-CA-C	-11.65	97.37	111.69
1	A	564	LYS	N-CA-C	-11.02	96.11	110.33
1	A	509	PHE	N-CA-C	10.19	126.96	113.72
1	A	172	ALA	N-CA-C	-10.04	101.59	114.04
1	A	561	ALA	N-CA-C	-8.61	98.93	110.55
1	A	64	LYS	N-CA-C	8.49	121.49	110.53
1	B	542	GLU	N-CA-C	-8.10	104.00	114.04
1	A	117	ARG	CA-C-N	7.84	129.64	119.84
1	A	117	ARG	C-N-CA	7.84	129.64	119.84
1	A	250	LEU	N-CA-C	7.71	119.77	111.36
1	B	440	HIS	CA-C-N	7.02	126.99	119.76
1	B	440	HIS	C-N-CA	7.02	126.99	119.76
1	B	511	ALA	N-CA-C	-6.85	104.89	113.18
1	B	168	CYS	N-CA-C	6.74	118.63	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	281	LYS	CA-C-N	6.38	127.81	119.84
1	A	281	LYS	C-N-CA	6.38	127.81	119.84
1	A	440	HIS	CA-C-N	6.34	126.37	119.90
1	A	440	HIS	C-N-CA	6.34	126.37	119.90
1	B	440	HIS	N-CA-C	6.25	123.63	109.81
1	A	100	GLU	N-CA-C	-6.25	103.75	111.75
1	B	146	HIS	CA-C-N	6.03	125.73	119.82
1	B	146	HIS	C-N-CA	6.03	125.73	119.82
1	B	449	ALA	N-CA-C	5.98	117.67	111.03
1	A	117	ARG	N-CA-C	5.91	119.95	108.85
1	B	523	ILE	N-CA-C	-5.86	103.76	111.09
1	B	479	GLU	N-CA-C	5.85	117.34	110.97
1	B	549	ASP	N-CA-C	-5.85	104.91	111.28
1	A	400	GLU	N-CA-C	5.80	117.60	111.28
1	B	49	PHE	N-CA-C	-5.77	98.51	110.80
1	A	94	GLN	N-CA-C	5.72	117.36	109.29
1	A	411	TYR	N-CA-C	5.56	118.10	111.71
1	A	449	ALA	N-CA-C	5.56	117.20	111.03
1	B	103	LEU	N-CA-C	-5.55	104.25	111.02
1	A	45	GLU	N-CA-C	-5.51	104.66	111.33
1	B	400	GLU	N-CA-C	5.47	117.32	111.36
1	A	104	GLN	OE1-CD-NE2	5.46	128.06	122.60
1	B	204	GLN	N-CA-C	5.40	117.24	111.36
1	A	16	GLU	N-CA-C	5.39	116.84	111.07
1	A	540	THR	CA-C-N	-5.33	111.36	121.54
1	A	540	THR	C-N-CA	-5.33	111.36	121.54
1	B	21	ALA	N-CA-C	-5.26	104.98	111.40
1	B	498	VAL	N-CA-C	5.23	112.73	107.55
1	B	445	ARG	N-CA-C	5.17	116.60	111.07
1	B	539	ALA	N-CA-C	5.09	121.64	110.80
1	B	538	LYS	N-CA-C	5.03	121.52	110.80
1	A	204	GLN	N-CA-C	5.03	116.84	111.36
1	A	61	ASN	N-CA-C	-5.00	105.50	112.30

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	4470	0	4271	260	0
1	B	4480	0	4303	186	0
2	A	26	0	36	7	0
2	B	26	0	36	4	0
3	A	60	0	0	13	0
3	B	60	0	0	8	0
All	All	9122	0	8646	447	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 (447) 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:97:GLU:C	1:A:99:ASN:H	1.50	1.11
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: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:97:GLU:C	1:A:99:ASN:N	2.18	0.96
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:OE1	1:B:571:GLU:HA	1.88	0.72
1:A:87:MET:HE1	1:A:105:HIS:HB3	1.70	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:A:98:ARG:HH11	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
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:A:325:VAL:HG12	1:A:329:MET:HE2	1.81	0.63
1:B:90:CYS:O	1:B:98:ARG:HG3	2.00	0.62
1:A:6:GLU:O	1:A:9:HIS:N	2.33	0.62
1:A:511:ALA:HB2	1:A:565:GLU:CB	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD13	1:A:66:LEU:H	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
1:A:178:LEU:O	1:A:179:LEU:C	2.43	0.60
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:OD1	1:A:471:ASP:N	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:B:511:ALA:C	1:B:513:ILE:H	2.08	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:B:118:PRO:HD2	1:B:123:MET:HE3	1.84	0.59
1:A:152:PRO:HB2	1:A:257:ARG:NH1	2.10	0.59
1:A:564:LYS:C	1:A:566:THR:H	2.09	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:A:366:PRO:C	1:A:368:GLU:N	2.60	0.58
1:B:485:ARG:HB3	1:B:486:PRO:HD3	1.85	0.58
1:A:563:ASP:CG	1:A:564:LYS:O	2.46	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:A:41:LYS:NZ	1:A:45:GLU:OE2	2.30	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:B:483:ASN:C	1:B:486:PRO:HD2	2.29	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:19:PHE:CD1	1:B:19:PHE:C	2.82	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:PRO:C	1:A:368:GLU:H	2.12	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:29:GLN:HG2	1:A:147:PRO:HA	1.88	0.56
1:B:370:TYR:CD1	1:B:370:TYR:C	2.84	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:117:ARG:HB2	1:A:123:MET:HE3	1.89	0.55
1:A:283:LEU:CG	1:A:284:LEU:N	2.68	0.55
1:A:168:CYS:SG	1:A:177:CYS:C	2.90	0.55
1:A:199:LYS:HG2	1:A:211:PHE:HE2	1.72	0.55
1:A:563:ASP:C	1:A:564:LYS:O	2.42	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
1:A:97:GLU:O	1:A:98:ARG:C	2.49	0.54
1:A:401:TYR:HE1	3:A:2060:HOH:O	1.88	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:B:240:LYS:HE2	1:B:244:GLU:OE2	2.07	0.54
1:A:564:LYS:C	1:A:566:THR:N	2.66	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:511:ALA:C	1:B:513:ILE:N	2.66	0.53
1:B:325:VAL:HG12	1:B:329:MET:CE	2.38	0.53
1:A:485:ARG:CZ	1:A:486:PRO:HD3	2.38	0.53
1:A:532:LEU:HG	2:A:4002:PFL:C8	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:A:370:TYR:CD1	1:A:370:TYR:C	2.87	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:66:LEU:HD21	3:A:2001:HOH:O	2.08	0.53
1:A:218:ARG:NH2	3:A:2017:HOH:O	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:508:THR:CG2	1:A:510:HIS:CE1	2.92	0.53
1:A:49:PHE:CD1	1:A:49:PHE:C	2.87	0.52
1:A:49:PHE:HE1	1:A:62:CYS:SG	2.31	0.52
1:A:178:LEU:HG	1:A:182:LEU:HG	1.91	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:27:PHE:CE2	1:A:74:LEU:HG	2.45	0.52
1:A:485:ARG:NH2	1:A:486:PRO:HG3	2.25	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:87:MET:HE1	1:A:105:HIS:CB	2.38	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: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
1:A:61:ASN:C	1:A:63:ASP:N	2.69	0.51
1:A:383:GLU:HB3	1:A:384:PRO:HD3	1.92	0.51
1:B:54:VAL:HG12	1:B:55:ALA:N	2.25	0.51
1:B:87:MET:HE1	1:B:105:HIS:HB3	1.92	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
2:A:4001:PFL:H111	3:A:2036:HOH:O	2.11	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:99:ASN:O	1:A:100:GLU:C	2.54	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:57:GLU:OE1	1:B:57:GLU:HA	2.10	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: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:34:CYS:HB3	1:A:39:HIS:HE2	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:61:ASN:HB3	1:B:64:LYS:HE2	1.94	0.49
1:B:373:VAL:HG13	1:B:374:PHE:HD1	1.78	0.49
1:B:441:PRO:C	1:B:443:ALA:N	2.70	0.49
1:A:49:PHE:C	1:A:49:PHE:HD1	2.20	0.49
1:A:511:ALA:CB	1:A:565:GLU:HG3	2.43	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:61:ASN:C	1:A:63:ASP:H	2.20	0.49
1:B:9:HIS:NE2	1:B:13:ASP:OD2	2.45	0.49
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:95:GLU:O	1:A:96:PRO:C	2.53	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:555:VAL:O	1:B:556:GLU:C	2.56	0.48
1:A:78:ALA:C	1:A:80:LEU:H	2.21	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:283:LEU:C	1:A:283:LEU:HD12	2.39	0.48
1:A:464:HIS:HE1	1:A:469:VAL:H	1.62	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:51:LYS:C	1:B:53:CYS:H	2.21	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:6:GLU:C	1:A:8:ALA:N	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:PHE:HE1	1:A:53:CYS:SG	2.37	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:B:100:GLU:O	1:B:104:GLN:CG	2.61	0.47
1:A:38:ASP:N	1:A:38:ASP:OD1	2.46	0.47
1:A:64:LYS:HB2	1:A:69:LEU:HD21	1.96	0.47
1:A:127:PHE:CE1	1:A:131:GLU:HG3	2.49	0.47
1:A:541:LYS:C	1:A:542:GLU:HG3	2.40	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:98:ARG:NH1	1:A:99:ASN:CB	2.78	0.47
1:A:279:CYS:HA	1:A:286:LYS:CD	2.42	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:B:37:GLU:CD	1:B:37:GLU:H	2.23	0.47
1:B:103:LEU:C	1:B:105:HIS:H	2.22	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:B:178:LEU:O	1:B:179:LEU:C	2.58	0.47
1:A:366:PRO:O	1:A:367:HIS:C	2.57	0.47
1:B:540:THR:HB	1:B:544:LEU:HG	1.98	0.47
1:A:5:SER:HB2	1:A:57:GLU:HG2	1.98	0.46
1:B:168:CYS:SG	1:B:177:CYS:C	2.98	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:99:ASN:C	1:A:101:CYS:N	2.69	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:A:283:LEU:O	1:A:284:LEU:C	2.59	0.46
1:B:464:HIS:CE1	1:B:469:VAL:H	2.34	0.46
1:A:66:LEU:HB3	1:A:70:PHE:HE2	1.78	0.46
1:A:420:THR:HG23	1:A:530:VAL:HG11	1.96	0.46
1:B:290:ILE:O	1:B:293:VAL:HG12	2.15	0.46
1:A:49:PHE:HD1	1:A:49:PHE:O	1.98	0.46
1:A:97:GLU:HA	1:A:98:ARG:HH12	1.79	0.46
1:A:410:ARG:CD	3:A:2035:HOH:O	1.97	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:B:85:GLY:C	1:B:87:MET:H	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:HIS:CB	1:A:98:ARG:HH21	2.27	0.46
1:A:81:ARG:CA	1:A:85:GLY:HA2	2.46	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:93:LYS:HB2	1:A:98:ARG:HA	1.98	0.45
1:A:306:ALA:CA	1:A:310:VAL:HG22	2.41	0.45
1:A:566:THR:C	1:A:568:PHE:N	2.70	0.45
1:A:538:LYS:O	1:A:539:ALA:C	2.59	0.45
1:A:37:GLU:CD	1:A:37:GLU:H	2.23	0.45
1:B:556:GLU:CG	1:B:557:LYS:H	2.25	0.45
1:A:222:ARG:C	1:A:224:PRO:HD3	2.41	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:563:ASP:O	1:A:564:LYS:C	2.59	0.45
1:A:503:ASN:C	1:A:503:ASN:ND2	2.75	0.45
1:B:57:GLU:HB3	1:B:58:SER:H	1.57	0.45
1:B:510:HIS:CB	1:B:512:ASP:OD1	2.65	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:6:GLU:O	1:A:8:ALA:N	2.49	0.45
1:A:7:VAL:CG2	1:A:66:LEU:HD12	2.47	0.45
1:A:378:LYS:HB3	1:A:379:PRO:CD	2.42	0.45
1:B:393:GLU:HA	1:B:396:GLU:HG3	1.98	0.45
1:A:78:ALA:C	1:A:80:LEU:N	2.74	0.44
1:B:370:TYR:C	1:B:370:TYR:HD1	2.24	0.44
1:B:570:GLU:O	1:B:574:LYS:HE3	2.17	0.44
1:A:66:LEU:N	1:A:66:LEU:CD1	2.78	0.44
1:A:419:SER:HB2	1:A:421:PRO:HD2	1.98	0.44
1:B:34:CYS:HB3	1:B:39:HIS:CD2	2.51	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:551:PHE:O	1:B:555:VAL:HG23	2.16	0.44
1:A:109:ASN:HD22	1:A:109:ASN:HA	1.68	0.44
1:B:529:LEU:HB2	1:B:548:MET:HE2	1.99	0.44
1:A:522:GLN:CA	3:A:2060:HOH:O	2.65	0.44
1:B:441:PRO:C	1:B:443:ALA:H	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:38:ASP:O	1:A:42:LEU:HG	2.17	0.44
1:A:280:GLU:HA	1:A:280:GLU:OE1	2.17	0.44
1:A:360:CYS:SG	1:A:370:TYR:N	2.91	0.44
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: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:B:283:LEU:CG	1:B:284:LEU:N	2.82	0.43
1:A:6:GLU:O	1:A:7:VAL:C	2.62	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:370:TYR:C	1:A:370:TYR:HD1	2.26	0.43
1:A:434:GLY:O	1:A:438:CYS:HB2	2.18	0.43
1:B:57:GLU:O	1:B:59:ALA:N	2.52	0.43
1:B:272:SER:HB3	1:B:275:LEU:HG	2.01	0.43
1:A:543:GLN:H	1:A:543:GLN:HG2	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:A:541:LYS:C	1:A:542:GLU:CG	2.92	0.43
1:B:85:GLY:C	1:B:87:MET:N	2.77	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
1:B:342:SER:OG	1:B:344:VAL:HG23	2.19	0.42
1:B:78:ALA:C	1:B:80:LEU:H	2.26	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:117:ARG:HA	1:B:118:PRO:HD3	1.86	0.42
1:B:70:PHE:N	1:B:70:PHE:CD1	2.88	0.42
1:B:185:LEU:HD23	1:B:185:LEU:HA	1.90	0.42
1:B:572:GLY:O	1:B:576:VAL:HG23	2.20	0.42
1:A:319:TYR:CE1	1:A:323:LYS:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:CYS:HB3	1:B:39:HIS:HE2	1.82	0.42
1:B:283:LEU:HD12	1:B:283:LEU:C	2.44	0.42
1:B:22:LEU:HD21	1:B:155:LEU:HD11	2.01	0.42
1:B:98:ARG:O	1:B:101:CYS:HB3	2.20	0.42
1:A:5:SER:CB	1:A:57:GLU:HG2	2.50	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:94:GLN:O	1:B:97:GLU:HB2	2.20	0.42
1:B:137:LYS:O	1:B:141:GLU:HG2	2.19	0.42
1:A:231:VAL:O	1:A:235:VAL:HG23	2.20	0.41
1:A:493:VAL:O	1:A:493:VAL:HG22	2.20	0.41
1:A:214:TRP:CD1	1:A:343:VAL:HG11	2.55	0.41
1:A:410:ARG:NH2	2:A:4001:PFL:C12	2.83	0.41
1:B:366:PRO:C	1:B:368:GLU:N	2.78	0.41
1:B:532:LEU:HD23	1:B:532:LEU:HA	1.87	0.41
1:A:247:HIS:CD2	1:A:247:HIS:O	2.73	0.41
1:B:503:ASN:OD1	1:B:503:ASN:C	2.63	0.41
1:B:522:GLN:HA	1:B:525:LYS:HB2	2.02	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:7:VAL:HG21	1:A:69:LEU:HD13	2.03	0.41
1:A:41:LYS:O	1:A:45:GLU:HG3	2.21	0.41
1:A:415:VAL:HG23	1:A:415:VAL:O	2.21	0.41
1:A:511:ALA:CB	1:A:565:GLU:CB	2.97	0.41
1:B:278:CYS:HB3	1:B:289:CYS:HB3	1.95	0.41
1:B:329:MET:HE3	1:B:329:MET:HB2	1.97	0.41
1:A:16:GLU:O	1:A:20:LYS:HB2	2.21	0.41
1:A:17:GLU:HA	1:A:17:GLU:OE1	2.21	0.41
1:A:302:LEU:HD23	1:A:302:LEU:HA	1.95	0.41
1:A:333:GLU:OE1	1:A:336:ARG:HD3	2.21	0.41
1:B:64:LYS:HE2	1:B:69:LEU:CD2	2.51	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:A:67:HIS:CE1	1:A:99:ASN:ND2	2.89	0.41
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:B:51:LYS:C	1:B:53:CYS:N	2.78	0.40
1:A:360:CYS:SG	1:A:369:CYS:C	3.05	0.40
1:A:398:LEU:H	1:A:398:LEU:HG	1.75	0.40
1:B:113:PRO:O	1:B:145:ARG:NH2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:LEU:HB2	1:B:180:PRO:HD3	2.03	0.40
1:A:87:MET:HE1	1:A:105:HIS:CG	2.57	0.40
1:A:566:THR:O	1:A:567:CYS:C	2.63	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:103:LEU:C	1:B:105:HIS:N	2.79	0.40
1:B:153:GLU:O	1:B:157:PHE:HD1	2.02	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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	4	3
1	B	576/585 (98%)	513 (89%)	49 (8%)	14 (2%)	4	3
All	All	1152/1170 (98%)	1016 (88%)	108 (9%)	28 (2%)	4	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

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Mol	Chain	Res	Type
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%)	413 (87%)	61 (13%)	4	4
1	B	475/511 (93%)	415 (87%)	60 (13%)	4	4
All	All	949/1022 (93%)	828 (87%)	121 (13%)	4	4

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	TYR

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Mol	Chain	Res	Type
1	A	37	GLU
1	A	38	ASP
1	A	47	THR
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	104	GLN
1	A	109	ASN
1	A	124	CYS
1	A	166	THR
1	A	174	LYS
1	A	179	LEU
1	A	195	LYS
1	A	212	LYS
1	A	222	ARG
1	A	232	SER
1	A	233	LYS
1	A	236	THR
1	A	245	CYS
1	A	249	ASP
1	A	252	GLU
1	A	268	GLN
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	305	LEU
1	A	317	LYS
1	A	323	LYS
1	A	329	MET
1	A	366	PRO
1	A	375	ASP
1	A	398	LEU
1	A	414	LYS
1	A	435	SER

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Mol	Chain	Res	Type
1	A	441	PRO
1	A	444	LYS
1	A	445	ARG
1	A	467	THR
1	A	471	ASP
1	A	482	VAL
1	A	486	PRO
1	A	493	VAL
1	A	498	VAL
1	A	500	LYS
1	A	503	ASN
1	A	508	THR
1	A	513	ILE
1	A	532	LEU
1	A	543	GLN
1	A	550	ASP
1	A	555	VAL
1	A	568	PHE
1	B	19	PHE
1	B	33	GLN
1	B	34	CYS
1	B	38	ASP
1	B	47	THR
1	B	56	ASP
1	B	57	GLU
1	B	58	SER
1	B	64	LYS
1	B	77	VAL
1	B	79	THR
1	B	82	GLU
1	B	83	THR
1	B	93	LYS
1	B	105	HIS
1	B	122	VAL
1	B	166	THR
1	B	174	LYS
1	B	179	LEU
1	B	204	GLN
1	B	209	ARG
1	B	212	LYS
1	B	222	ARG
1	B	232	SER

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Mol	Chain	Res	Type
1	B	233	LYS
1	B	249	ASP
1	B	262	LYS
1	B	269	ASP
1	B	276	LYS
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	329	MET
1	B	337	ARG
1	B	344	VAL
1	B	352	THR
1	B	375	ASP
1	B	392	CYS
1	B	398	LEU
1	B	414	LYS
1	B	435	SER
1	B	445	ARG
1	B	467	THR
1	B	480	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	555	VAL
1	B	564	LYS
1	B	566	THR
1	B	568	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	A	109	ASN

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Mol	Chain	Res	Type
1	A	130	ASN
1	A	196	GLN
1	A	247	HIS
1	A	268	GLN
1	A	295	ASN
1	A	367	HIS
1	A	385	GLN
1	A	464	HIS
1	A	503	ASN
1	A	535	HIS
1	A	543	GLN
1	B	33	GLN
1	B	67	HIS
1	B	99	ASN
1	B	196	GLN
1	B	204	GLN
1	B	385	GLN
1	B	464	HIS
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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	4001	-	13,13,13	1.86	6 (46%)	18,18,18	0.89	0
2	PFL	B	4002	-	13,13,13	1.54	4 (30%)	18,18,18	1.04	0
2	PFL	A	4002	-	13,13,13	1.72	4 (30%)	18,18,18	1.00	1 (5%)
2	PFL	A	4001	-	13,13,13	1.88	5 (38%)	18,18,18	0.87	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	4001	-	-	1/8/8/8	0/1/1/1
2	PFL	B	4002	-	-	0/8/8/8	0/1/1/1
2	PFL	A	4002	-	-	0/8/8/8	0/1/1/1
2	PFL	A	4001	-	-	1/8/8/8	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4001	PFL	C5-C6	3.33	1.43	1.39
2	B	4001	PFL	C5-C6	3.25	1.43	1.39
2	A	4002	PFL	C5-C6	3.16	1.43	1.39
2	B	4001	PFL	C1-C2	2.92	1.44	1.39
2	A	4001	PFL	C1-C2	2.89	1.44	1.39
2	B	4002	PFL	C1-C2	2.72	1.43	1.39
2	B	4002	PFL	C5-C6	2.65	1.43	1.39
2	B	4001	PFL	C3-C2	2.63	1.43	1.39
2	A	4001	PFL	C3-C2	2.58	1.42	1.39
2	A	4002	PFL	C3-C2	2.55	1.42	1.39
2	A	4002	PFL	C6-C10	2.43	1.55	1.52
2	B	4002	PFL	C6-C10	2.33	1.55	1.52
2	B	4001	PFL	O1-C1	2.24	1.42	1.36
2	B	4002	PFL	C3-C2	2.23	1.42	1.39
2	A	4001	PFL	O1-C1	2.22	1.42	1.36
2	A	4001	PFL	C6-C10	2.10	1.55	1.52
2	B	4001	PFL	C6-C10	2.08	1.55	1.52
2	B	4001	PFL	C1-C6	2.04	1.42	1.39
2	A	4002	PFL	C1-C2	2.03	1.42	1.39

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	4002	PFL	C3-C2-C7	2.26	123.08	119.83

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	4001	PFL	C3-C2-C7-C9
2	A	4001	PFL	C3-C2-C7-C9

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	4002	PFL	4	0
2	A	4002	PFL	3	0
2	A	4001	PFL	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

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%)	0.82	77 (13%) 7 5	18, 54, 105, 121	0
1	B	578/585 (98%)	0.85	81 (14%) 6 4	22, 57, 113, 129	0
All	All	1156/1170 (98%)	0.84	158 (13%) 6 5	18, 56, 110, 129	0

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	539	ALA	8.6
1	B	539	ALA	6.3
1	B	582	ALA	4.7
1	A	96	PRO	4.6
1	B	554	PHE	4.5
1	B	566	THR	4.4
1	A	55	ALA	4.3
1	A	87	MET	4.1
1	B	540	THR	4.1
1	A	84	TYR	3.9
1	B	84	TYR	3.9
1	B	553	ALA	3.8
1	A	56	ASP	3.8
1	A	7	VAL	3.8
1	B	87	MET	3.7
1	B	562	ASP	3.7
1	B	300	ALA	3.7
1	A	558	CYS	3.7
1	A	165	PHE	3.6
1	A	566	THR	3.6
1	B	561	ALA	3.6
1	A	65	SER	3.6
1	A	90	CYS	3.6
1	B	54	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	88	ALA	3.5
1	B	78	ALA	3.5
1	A	561	ALA	3.5
1	A	560	LYS	3.4
1	A	50	ALA	3.4
1	A	553	ALA	3.4
1	B	103	LEU	3.4
1	A	66	LEU	3.4
1	A	563	ASP	3.4
1	A	554	PHE	3.4
1	B	102	PHE	3.4
1	B	575	LEU	3.3
1	B	516	LEU	3.3
1	A	582	ALA	3.3
1	B	513	ILE	3.3
1	A	567	CYS	3.2
1	B	514	CYS	3.2
1	B	7	VAL	3.2
1	A	575	LEU	3.2
1	A	179	LEU	3.1
1	A	72	ASP	3.1
1	B	563	ASP	3.1
1	B	581	ALA	3.1
1	B	90	CYS	3.0
1	B	74	LEU	3.0
1	B	565	GLU	3.0
1	A	572	GLY	3.0
1	A	76	THR	3.0
1	A	164	ALA	3.0
1	B	275	LEU	2.9
1	B	564	LYS	2.9
1	A	168	CYS	2.9
1	B	76	THR	2.9
1	B	558	CYS	2.8
1	B	96	PRO	2.8
1	A	568	PHE	2.8
1	A	516	LEU	2.8
1	B	30	TYR	2.8
1	A	8	ALA	2.8
1	B	50	ALA	2.8
1	B	467	THR	2.7
1	B	580	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	83	THR	2.7
1	A	11	PHE	2.6
1	B	469	VAL	2.6
1	A	73	LYS	2.6
1	B	92	ALA	2.6
1	A	301	ASP	2.6
1	A	540	THR	2.6
1	B	47	THR	2.6
1	A	169	CYS	2.6
1	A	57	GLU	2.6
1	B	59	ALA	2.6
1	A	52	THR	2.6
1	A	68	THR	2.6
1	B	507	PHE	2.6
1	B	568	PHE	2.6
1	A	91	CYS	2.5
1	B	301	ASP	2.5
1	B	247	HIS	2.5
1	B	538	LYS	2.5
1	A	103	LEU	2.5
1	A	283	LEU	2.5
1	B	567	CYS	2.5
1	A	565	GLU	2.5
1	B	548	MET	2.5
1	B	537	PRO	2.5
1	A	102	PHE	2.5
1	B	5	SER	2.5
1	A	123	MET	2.5
1	A	82	GLU	2.4
1	A	83	THR	2.4
1	B	52	THR	2.4
1	B	541	LYS	2.4
1	B	79	THR	2.4
1	B	515	THR	2.4
1	A	513	ILE	2.4
1	B	552	ALA	2.4
1	A	79	THR	2.4
1	A	310	VAL	2.4
1	B	14	LEU	2.4
1	B	69	LEU	2.4
1	B	56	ASP	2.3
1	A	78	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	54	VAL	2.3
1	B	91	CYS	2.3
1	B	57	GLU	2.3
1	A	247	HIS	2.3
1	B	77	VAL	2.3
1	B	502	PHE	2.3
1	B	560	LYS	2.3
1	A	507	PHE	2.3
1	A	509	PHE	2.3
1	A	576	VAL	2.3
1	B	468	PRO	2.3
1	A	577	ALA	2.3
1	B	578	ALA	2.3
1	A	541	LYS	2.3
1	A	70	PHE	2.2
1	A	300	ALA	2.2
1	B	577	ALA	2.2
1	A	174	LYS	2.2
1	B	519	LYS	2.2
1	A	69	LEU	2.2
1	B	547	VAL	2.2
1	A	59	ALA	2.2
1	A	569	ALA	2.2
1	B	557	LYS	2.2
1	B	11	PHE	2.2
1	B	60	GLU	2.2
1	B	164	ALA	2.2
1	A	549	ASP	2.2
1	A	562	ASP	2.2
1	A	559	CYS	2.2
1	A	5	SER	2.2
1	B	511	ALA	2.2
1	B	179	LEU	2.1
1	A	156	PHE	2.1
1	B	68	THR	2.1
1	B	466	LYS	2.1
1	B	555	VAL	2.1
1	B	156	PHE	2.1
1	A	99	ASN	2.1
1	B	127	PHE	2.1
1	B	73	LYS	2.1
1	B	504	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	85	GLY	2.1
1	A	81	ARG	2.1
1	A	564	LYS	2.0
1	A	94	GLN	2.0
1	B	98	ARG	2.0
1	A	515	THR	2.0
1	B	170	GLN	2.0
1	A	499	PRO	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	PFL	B	4001	13/13	0.81	0.22	65,68,71,72	0
2	PFL	A	4001	13/13	0.86	0.17	60,62,66,67	0
2	PFL	B	4002	13/13	0.86	0.14	87,88,89,90	0
2	PFL	A	4002	13/13	0.88	0.15	76,77,79,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.