



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:05 PM UTC

PDB ID : 4F5S / pdb_00004f5s
Title : Crystal Structure of Bovine Serum Albumin
Authors : Bujacz, A.; Bujacz, G.
Deposited on : 2012-05-13
Resolution : 2.47 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

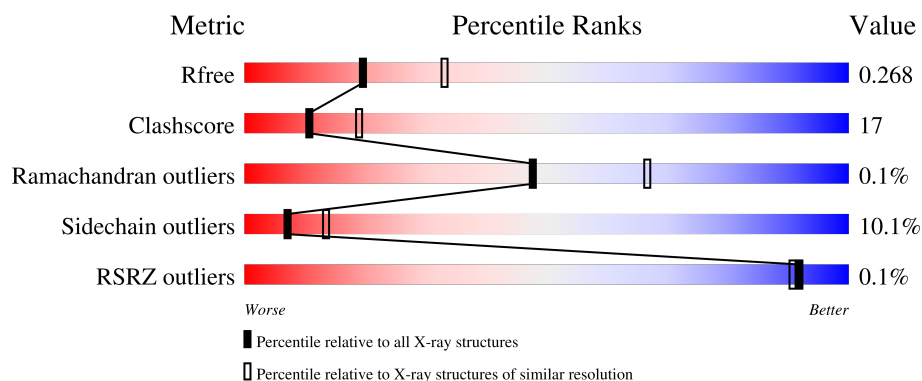
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.47 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))
R_{free}	180053	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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	583	57% 37% 5%
1	B	583	62% 32% 6%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9675 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.

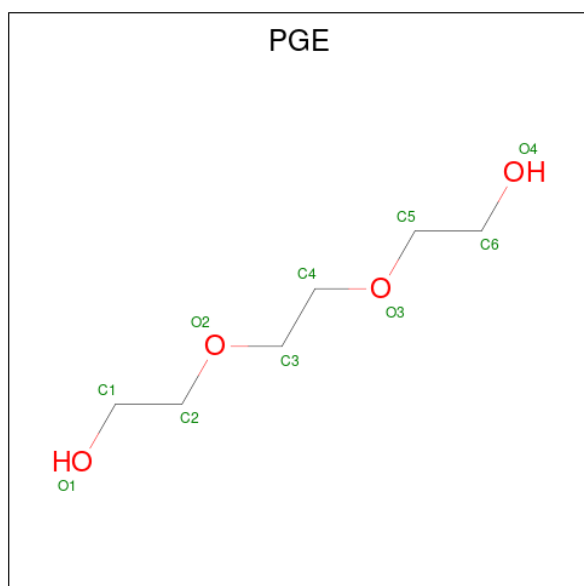
- Molecule 1 is a protein called Serum albumin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	583	Total	C	N	O	S	0	3	0
			4672	2947	787	899	39			
1	B	583	Total	C	N	O	S	0	2	0
			4666	2943	784	900	39			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	190	THR	ALA	variant	UNP P02769
B	190	THR	ALA	variant	UNP P02769

- Molecule 2 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	6	4		

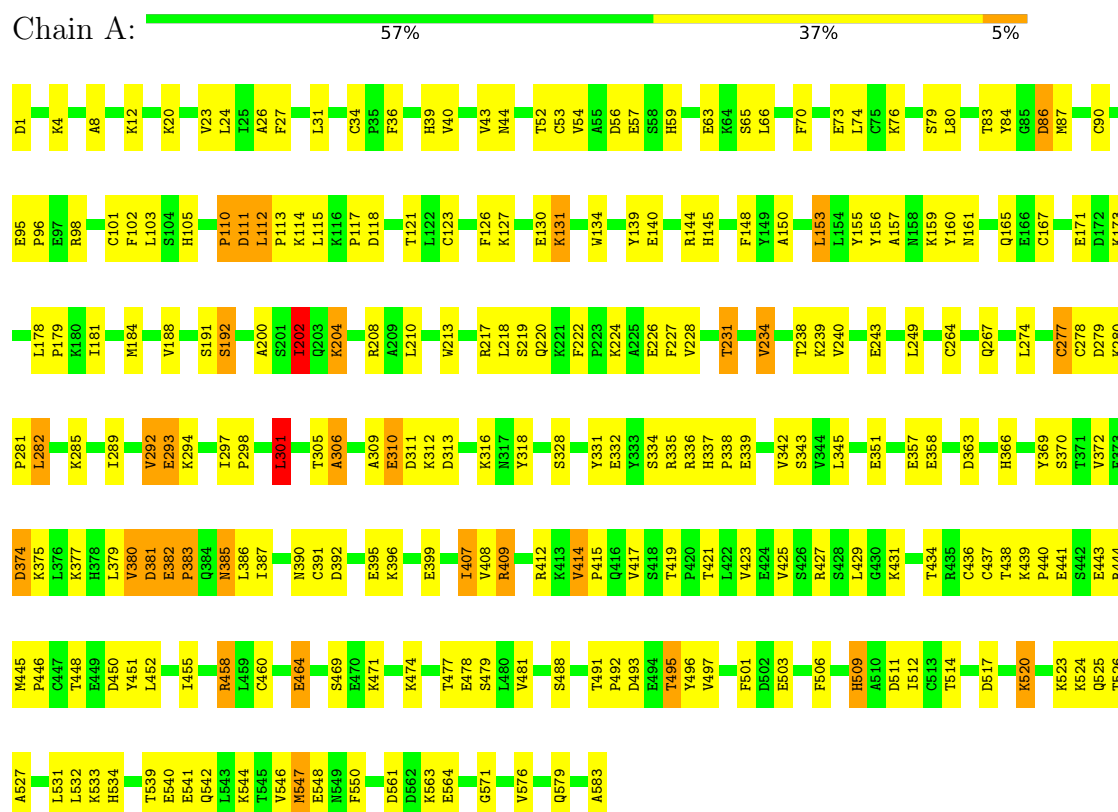
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	166	Total 166	O 166	0	0
3	B	161	Total 161	O 161	0	0

3 Residue-property plots

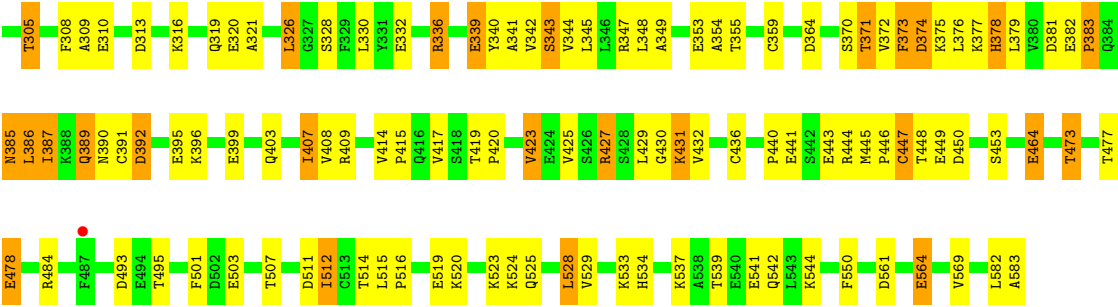
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	217.80Å 44.99Å 143.06Å 90.00° 114.13° 90.00°	Depositor
Resolution (Å)	40.00 – 2.47 40.00 – 2.47	Depositor EDS
% Data completeness (in resolution range)	94.6 (40.00-2.47) 94.6 (40.00-2.47)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.197 , 0.259 0.210 , 0.268	Depositor DCC
R_{free} test set	1436 reflections (3.11%)	wwPDB-VP
Wilson B-factor (Å ²)	64.4	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9675	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% 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: PGE

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	1.22	8/4776 (0.2%)	1.36	36/6446 (0.6%)
1	B	1.13	4/4767 (0.1%)	1.36	34/6435 (0.5%)
All	All	1.18	12/9543 (0.1%)	1.36	70/12881 (0.5%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	432	VAL	N-CA	6.69	1.54	1.46
1	B	142	ALA	CA-CB	-6.17	1.43	1.53
1	A	240	VAL	CA-CB	5.99	1.61	1.54
1	A	103	LEU	N-CA	5.97	1.53	1.46
1	A	101	CYS	C-O	-5.58	1.17	1.24
1	A	488	SER	C-O	-5.56	1.17	1.24
1	A	150	ALA	CA-CB	-5.46	1.44	1.53
1	A	191	SER	N-CA	-5.43	1.39	1.46
1	B	528	LEU	C-O	-5.40	1.17	1.24
1	A	547	MET	CG-SD	5.09	1.93	1.80
1	A	423	VAL	CA-CB	5.07	1.61	1.54
1	B	523	LYS	C-O	-5.06	1.17	1.24

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	LYS	N-CA-C	12.77	125.28	111.36
1	B	564	GLU	N-CA-C	-11.33	98.91	111.14
1	B	478	GLU	N-CA-C	10.73	122.72	111.14
1	B	227	PHE	N-CA-C	9.98	121.75	111.07
1	B	423	VAL	N-CA-C	-9.74	101.37	110.53
1	B	436	CYS	N-CA-C	8.43	126.64	114.16
1	B	86	ASP	N-CA-C	-8.09	104.55	114.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	473	THR	N-CA-C	-8.06	102.57	111.36
1	A	112	LEU	CA-C-N	7.97	128.03	119.90
1	A	112	LEU	C-N-CA	7.97	128.03	119.90
1	A	382	GLU	CA-C-N	7.86	127.42	119.24
1	A	382	GLU	C-N-CA	7.86	127.42	119.24
1	A	306	ALA	N-CA-C	6.85	119.33	111.11
1	A	277	CYS	N-CA-C	6.77	120.64	112.38
1	B	347	ARG	N-CA-C	-6.71	104.35	112.54
1	B	141	ILE	CB-CA-C	-6.62	103.60	111.94
1	B	111	ASP	N-CA-C	6.62	120.37	111.24
1	A	110	PRO	N-CA-C	6.57	122.12	114.03
1	B	167	CYS	N-CA-C	6.54	119.73	111.69
1	B	383	PRO	CB-CA-C	-6.52	102.16	111.68
1	B	181	ILE	N-CA-C	6.50	117.13	110.82
1	A	292	VAL	N-CA-C	6.47	118.40	109.80
1	A	222	PHE	CA-C-N	6.45	126.14	119.82
1	A	222	PHE	C-N-CA	6.45	126.14	119.82
1	A	34	CYS	N-CA-C	6.37	117.73	109.64
1	A	495	THR	N-CA-C	-6.24	104.14	112.94
1	A	202	ILE	CB-CA-C	-6.20	103.90	112.02
1	B	305	THR	N-CA-C	6.19	119.93	112.38
1	B	383	PRO	N-CA-C	6.12	121.50	113.86
1	A	386	LEU	N-CA-C	-6.09	104.33	110.97
1	A	414	VAL	CA-C-N	6.08	125.96	119.28
1	A	414	VAL	C-N-CA	6.08	125.96	119.28
1	A	167	CYS	N-CA-C	6.07	120.85	112.90
1	B	242	LYS	N-CA-C	-6.02	104.63	111.07
1	B	271	SER	N-CA-C	5.96	118.20	108.55
1	B	216	ALA	N-CA-C	5.93	117.54	111.14
1	B	91	CYS	N-CA-C	5.88	119.98	112.34
1	A	278	CYS	N-CA-C	-5.85	105.96	112.57
1	B	478	GLU	CB-CA-C	-5.84	101.67	110.90
1	B	427	ARG	N-CA-C	-5.83	104.84	111.14
1	B	425	VAL	N-CA-C	5.71	115.90	110.42
1	B	299	GLU	N-CA-C	5.71	118.71	111.69
1	B	141	ILE	N-CA-C	-5.67	105.57	111.58
1	A	455	ILE	N-CA-C	-5.64	105.60	111.58
1	A	301	LEU	CA-C-N	5.53	126.08	120.38
1	A	301	LEU	C-N-CA	5.53	126.08	120.38
1	A	546	VAL	N-CA-C	5.45	115.65	110.42
1	B	373	PHE	N-CA-C	5.39	117.91	111.71
1	A	380	VAL	CB-CA-C	-5.38	104.19	112.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	145	HIS	CA-C-N	-5.37	115.35	120.83
1	A	145	HIS	C-N-CA	-5.37	115.35	120.83
1	A	363	ASP	N-CA-C	5.35	117.11	111.28
1	B	52	THR	N-CA-C	-5.35	105.61	111.82
1	A	277	CYS	N-CA-CB	-5.32	101.27	110.32
1	A	380	VAL	N-CA-C	5.31	118.50	111.17
1	A	495	THR	N-CA-CB	-5.30	102.24	110.98
1	A	527	ALA	N-CA-C	-5.30	105.67	111.82
1	A	497	VAL	N-CA-C	-5.30	104.08	108.63
1	B	432	VAL	CB-CA-C	-5.29	105.10	112.04
1	B	74	LEU	N-CA-C	-5.26	105.46	111.14
1	A	576	VAL	N-CA-C	5.15	115.36	110.42
1	B	478	GLU	N-CA-CB	-5.15	102.61	110.07
1	B	228	VAL	N-CA-CB	-5.15	104.80	110.51
1	B	53	CYS	N-CA-C	-5.09	105.42	111.69
1	B	150	ALA	CA-C-N	-5.07	113.71	119.28
1	B	150	ALA	C-N-CA	-5.07	113.71	119.28
1	A	234	VAL	N-CA-C	5.04	115.26	110.53
1	B	478	GLU	CB-CG-CD	5.02	121.13	112.60
1	A	571	GLY	CA-C-N	5.01	124.62	119.05
1	A	571	GLY	C-N-CA	5.01	124.62	119.05

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	4672	0	4597	155	0
1	B	4666	0	4583	155	0
2	A	10	0	14	2	0
3	A	166	0	0	25	0
3	B	161	0	0	27	0
All	All	9675	0	9194	310	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 17.

All (310) 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:140:GLU:HG3	1:A:144:ARG:NH1	1.65	1.11
1:A:140:GLU:HG3	1:A:144:ARG:HH12	1.16	1.11
1:B:341:ALA:HB1	3:B:746:HOH:O	1.53	1.07
1:B:519:GLU:HG2	3:B:722:HOH:O	1.62	0.99
1:A:298:PRO:O	1:A:301:LEU:HD12	1.64	0.94
1:B:298:PRO:HG2	1:B:301:LEU:HD11	1.51	0.91
1:B:383:PRO:O	1:B:386:LEU:HD23	1.71	0.90
1:B:36:PHE:O	1:B:40:VAL:HG23	1.72	0.89
1:A:539:THR:OG1	1:A:542:GLN:HG3	1.73	0.89
1:B:503:GLU:HB3	3:B:749:HOH:O	1.73	0.87
1:B:84:TYR:HB3	1:B:87:MET:HG3	1.57	0.86
1:A:27:PHE:HB3	1:A:39:HIS:CD2	2.11	0.85
1:B:345:LEU:HA	1:B:348:LEU:HD12	1.60	0.83
1:A:298:PRO:O	1:A:301:LEU:CD1	2.27	0.83
1:A:493:ASP:HB2	3:A:864:HOH:O	1.80	0.82
1:A:436:CYS:O	1:A:444:ARG:HG2	1.81	0.80
1:A:391:CYS:O	1:A:395:GLU:HG2	1.82	0.80
1:B:215:VAL:HB	1:B:330:LEU:HD23	1.65	0.79
1:A:239:LYS:O	1:A:243:GLU:HG3	1.84	0.77
1:A:293:GLU:HG3	1:A:294:LYS:N	1.97	0.77
1:A:31:LEU:HD11	1:A:74:LEU:HD22	1.67	0.77
1:B:391:CYS:O	1:B:395:GLU:HG2	1.86	0.76
1:B:23:VAL:HG12	1:B:43:VAL:HG22	1.69	0.75
1:A:115:LEU:HD11	1:A:140:GLU:HG2	1.70	0.74
1:B:309:ALA:HB2	1:B:373:PHE:CE1	2.23	0.74
1:B:516:PRO:HD3	3:B:719:HOH:O	1.87	0.72
1:A:561:ASP:HB2	3:A:836:HOH:O	1.87	0.72
1:B:414:VAL:HG12	1:B:417:VAL:HG23	1.71	0.72
1:A:301:LEU:HB3	1:A:336:ARG:NH1	2.05	0.72
1:A:95:GLU:OE2	1:A:95:GLU:HA	1.90	0.71
1:B:158:ASN:ND2	1:B:283:LEU:HD12	2.05	0.71
1:B:297:ILE:HG13	3:B:754:HOH:O	1.90	0.71
1:A:210:LEU:O	1:A:213:TRP:HB3	1.90	0.71
1:A:86:ASP:OD2	1:A:105:HIS:NE2	2.23	0.71
1:A:39:HIS:CG	3:A:834:HOH:O	2.44	0.71
1:A:374:ASP:N	1:A:374:ASP:OD1	2.23	0.71
1:B:316:LYS:HG3	3:B:717:HOH:O	1.90	0.71
1:A:390:ASN:OD1	1:A:409:ARG:NH2	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:GLU:HA	1:B:444:ARG:HD3	1.73	0.70
1:A:293:GLU:HG3	1:A:294:LYS:H	1.57	0.70
1:B:427:ARG:HD2	1:B:525:GLN:OE1	1.91	0.70
1:A:23:VAL:HG12	1:A:43:VAL:HG22	1.74	0.69
1:B:46:LEU:HD21	1:B:73:GLU:HG3	1.74	0.69
1:B:271:SER:HA	1:B:295:ASP:OD2	1.91	0.69
1:A:503:GLU:H	1:A:503:GLU:CD	2.00	0.69
1:A:579:GLN:O	1:A:583:ALA:HB3	1.91	0.68
1:A:451:TYR:HD2	3:A:812:HOH:O	1.75	0.68
1:A:20:LYS:NZ	1:A:44:ASN:OD1	2.26	0.68
1:A:547:MET:HE1	3:A:862:HOH:O	1.93	0.68
1:A:218:LEU:HD12	1:A:234:VAL:HG23	1.75	0.67
1:A:445:MET:HB3	1:A:446:PRO:HD3	1.75	0.67
1:A:27:PHE:HB3	1:A:39:HIS:HD2	1.57	0.67
1:A:474:LYS:O	1:A:478:GLU:HB2	1.95	0.67
1:A:427:ARG:HD2	1:A:525:GLN:OE1	1.95	0.66
1:B:414:VAL:CG1	1:B:417:VAL:HG23	2.25	0.66
1:A:202:ILE:HD11	1:A:210:LEU:HD22	1.78	0.65
1:B:116:LYS:H	1:B:116:LYS:HD3	1.60	0.65
1:A:90:CYS:O	1:A:98:ARG:HG3	1.97	0.64
1:B:431:LYS:HD2	3:B:734:HOH:O	1.96	0.64
1:A:123:CYS:SG	1:A:173:LYS:HD2	2.38	0.64
1:A:471:LYS:NZ	1:A:491:THR:O	2.29	0.64
1:A:439:LYS:HD3	1:A:443:GLU:OE1	1.98	0.64
1:B:524:LYS:HG2	1:B:550:PHE:HE2	1.63	0.64
1:A:385:ASN:OD1	1:A:385:ASN:N	2.23	0.63
1:A:140:GLU:CG	1:A:144:ARG:HH12	2.02	0.63
1:A:495:THR:C	3:A:848:HOH:O	2.40	0.63
1:A:228:VAL:HA	1:A:231:THR:OG1	1.99	0.63
1:B:35:PRO:HB2	3:B:759:HOH:O	1.97	0.63
1:B:414:VAL:HG12	1:B:414:VAL:O	1.97	0.63
1:A:496:TYR:N	3:A:848:HOH:O	2.31	0.63
1:A:451:TYR:CD2	3:A:812:HOH:O	2.49	0.62
1:A:79:SER:O	1:A:83:THR:HB	1.98	0.62
1:B:132:LYS:HB2	3:B:707:HOH:O	1.99	0.62
1:B:81:ARG:HA	1:B:88:ALA:HB2	1.82	0.62
1:A:509:HIS:N	1:A:509:HIS:CD2	2.68	0.62
1:B:106:LYS:NZ	3:B:683:HOH:O	2.33	0.62
1:A:524:LYS:HG2	1:A:550:PHE:HE2	1.65	0.61
1:A:342:VAL:O	1:A:345:LEU:N	2.33	0.61
1:B:330:LEU:HD13	1:B:349:ALA:HB2	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:HIS:CD2	1:B:378:HIS:C	2.79	0.61
1:B:450:ASP:O	1:B:453:SER:HB3	2.00	0.61
1:A:544:LYS:O	1:A:548:GLU:HG3	1.99	0.61
1:A:381:ASP:OD1	1:A:381:ASP:N	2.32	0.61
1:A:382:GLU:HB3	1:A:383:PRO:HD3	1.83	0.60
1:B:106:LYS:HE2	1:B:146:PRO:O	2.02	0.60
1:B:134:TRP:HB2	1:B:161:ASN:HD21	1.66	0.60
1:B:30:TYR:HE1	1:B:103:LEU:HD23	1.66	0.60
1:B:200:ALA:O	1:B:204:LYS:HB2	2.01	0.60
1:B:106:LYS:HG2	1:B:146:PRO:HB2	1.84	0.59
1:B:484:ARG:HD2	1:B:484:ARG:C	2.27	0.59
1:A:126:PHE:O	1:A:130:GLU:HG3	2.03	0.59
1:B:382:GLU:HB2	1:B:383:PRO:HD3	1.84	0.59
1:B:389:GLN:O	1:B:392:ASP:HB2	2.02	0.58
1:A:155:TYR:CE1	1:A:159:LYS:HE3	2.39	0.58
1:B:520:LYS:HD2	3:B:679:HOH:O	2.02	0.58
1:B:223:PRO:HG2	1:B:295:ASP:HB3	1.84	0.58
1:B:37:ASP:HB2	3:B:759:HOH:O	2.03	0.58
1:B:342:VAL:O	1:B:343:SER:C	2.46	0.58
1:A:297:ILE:HG22	1:A:301:LEU:CD1	2.33	0.58
1:A:458:ARG:O	1:A:458:ARG:HG3	2.03	0.57
1:B:182:GLU:HG2	3:B:611:HOH:O	2.03	0.57
1:A:178:LEU:N	1:A:179:PRO:CD	2.67	0.57
1:B:415:PRO:O	1:B:533:LYS:HE2	2.04	0.57
1:A:311:ASP:C	1:A:313:ASP:H	2.11	0.57
1:B:374:ASP:OD1	1:B:374:ASP:N	2.37	0.57
1:A:309:ALA:O	1:A:369:TYR:HE2	1.86	0.57
1:B:160:TYR:O	1:B:164:PHE:HD2	1.87	0.57
1:B:537:LYS:HD3	3:B:731:HOH:O	2.05	0.57
1:A:228:VAL:HG23	3:A:814:HOH:O	2.05	0.57
1:A:153:LEU:HD12	1:A:153:LEU:O	2.06	0.56
1:B:514:THR:CG2	1:B:514:THR:O	2.54	0.56
1:A:87:MET:HE3	1:A:102:PHE:HD1	1.71	0.56
1:B:381:ASP:OD2	1:B:381:ASP:N	2.36	0.56
1:B:582:LEU:O	1:B:583:ALA:C	2.48	0.56
1:A:226:GLU:HG3	3:A:814:HOH:O	2.05	0.56
1:A:279:ASP:O	1:A:279:ASP:OD2	2.24	0.56
1:B:419:THR:HB	1:B:420:PRO:HD3	1.88	0.56
1:B:297:ILE:CG1	3:B:754:HOH:O	2.52	0.55
1:B:407:ILE:HG21	1:B:528:LEU:HG	1.88	0.55
1:B:514:THR:O	1:B:514:THR:HG22	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:ARG:NE	3:A:851:HOH:O	2.37	0.55
1:B:37:ASP:HA	1:B:40:VAL:HG23	1.89	0.54
1:B:271:SER:HB3	1:B:274:LEU:HG	1.89	0.54
1:A:220:GLN:HG2	1:A:338:PRO:HA	1.88	0.54
1:B:328:SER:O	1:B:332:GLU:HG2	2.08	0.54
1:A:39:HIS:CD2	3:A:834:HOH:O	2.61	0.54
1:A:95:GLU:OE2	1:A:96:PRO:HA	2.07	0.54
1:B:118:ASP:O	1:B:122:LEU:HG	2.08	0.54
1:A:399:GLU:OE1	1:A:434:THR:OG1	2.22	0.54
1:B:178:LEU:HB2	1:B:179:PRO:HD3	1.90	0.54
1:A:524:LYS:HG2	1:A:550:PHE:CE2	2.43	0.54
1:A:337:HIS:HA	1:A:339:GLU:OE1	2.08	0.54
1:A:372:VAL:O	1:A:375:LYS:HB2	2.08	0.53
1:B:309:ALA:HB2	1:B:373:PHE:HE1	1.73	0.53
1:B:299:GLU:N	3:B:758:HOH:O	2.40	0.53
1:A:52:THR:HG23	3:A:724:HOH:O	2.09	0.53
1:B:313:ASP:HA	3:B:717:HOH:O	2.08	0.53
1:A:481:VAL:HG22	1:A:481:VAL:O	2.09	0.52
1:A:506:PHE:HB3	2:A:601:PGE:H6	1.90	0.52
1:B:344:VAL:O	1:B:348:LEU:HG	2.10	0.52
1:B:226:GLU:OE1	1:B:226:GLU:HA	2.09	0.52
1:A:148:PHE:CD2	1:A:192:SER:HB2	2.45	0.52
1:B:336:ARG:HB3	3:B:709:HOH:O	2.10	0.52
1:B:167:CYS:HB3	1:B:177:LEU:HD12	1.91	0.52
1:B:444:ARG:O	1:B:448:THR:HG23	2.10	0.52
1:A:523:LYS:NZ	3:A:771:HOH:O	2.43	0.51
1:B:319:GLN:HA	1:B:319:GLN:NE2	2.26	0.51
1:B:71:GLY:HA2	1:B:74:LEU:HD12	1.92	0.51
1:B:321:ALA:HA	3:B:753:HOH:O	2.11	0.51
1:A:285:LYS:O	1:A:289:ILE:HG13	2.10	0.51
1:A:531:LEU:HD22	2:A:601:PGE:H4	1.91	0.51
1:B:248:ASP:HB3	1:B:251:GLU:CG	2.41	0.51
1:A:112:LEU:HB2	3:A:711:HOH:O	2.11	0.51
1:A:218:LEU:HD12	1:A:234:VAL:CG2	2.40	0.51
1:A:202:ILE:CD1	1:A:210:LEU:HD22	2.41	0.50
1:B:373:PHE:HA	1:B:376:LEU:HB2	1.93	0.50
1:B:445:MET:N	1:B:446:PRO:HD2	2.27	0.50
1:B:515:LEU:N	3:B:679:HOH:O	2.43	0.50
1:A:208:ARG:HB2	3:A:773:HOH:O	2.12	0.50
1:A:477:THR:HG22	3:A:776:HOH:O	2.11	0.50
1:B:151:PRO:HB2	1:B:256:ARG:HH11	1.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:ASP:HB3	1:B:251:GLU:CD	2.36	0.50
1:A:511:ASP:O	1:A:514:THR:N	2.42	0.50
1:B:126:PHE:HZ	1:B:165:GLN:CG	2.25	0.50
1:A:280:LYS:HB3	1:A:281:PRO:CD	2.42	0.50
1:A:73:GLU:OE1	1:A:76:LYS:NZ	2.45	0.50
1:B:158:ASN:HD21	1:B:283:LEU:HD12	1.76	0.50
1:A:382:GLU:HB3	1:A:383:PRO:CD	2.42	0.50
1:B:29:GLN:HG2	1:B:146:PRO:HA	1.94	0.50
1:B:67:HIS:NE2	1:B:248:ASP:OD1	2.40	0.50
1:B:111:ASP:OD1	1:B:111:ASP:O	2.30	0.49
1:B:537:LYS:HB2	3:B:755:HOH:O	2.12	0.49
1:A:26:ALA:HB2	1:A:249:LEU:HD12	1.94	0.49
1:A:56:ASP:OD2	1:A:59:HIS:HB2	2.13	0.49
1:A:412:ARG:HB3	1:A:492:PRO:HB3	1.94	0.49
1:B:140:GLU:OE1	1:B:144:ARG:NH1	2.35	0.49
1:B:232:LYS:HG3	3:B:624:HOH:O	2.13	0.49
1:A:115:LEU:O	1:A:117:PRO:HD3	2.13	0.49
1:B:407:ILE:CG2	1:B:528:LEU:HG	2.43	0.49
1:A:421:THR:O	1:A:425:VAL:HG23	2.13	0.49
1:B:501:PHE:HB2	1:B:534:HIS:CE1	2.48	0.48
1:B:213:TRP:HZ2	1:B:217:ARG:HH11	1.62	0.48
1:A:409:ARG:HD2	3:A:847:HOH:O	2.13	0.48
1:B:544:LYS:HG3	3:B:643:HOH:O	2.13	0.48
1:A:126:PHE:CE1	1:A:130:GLU:HG2	2.49	0.48
1:B:26:ALA:HB2	1:B:249:LEU:HD12	1.96	0.48
1:B:383:PRO:HG2	1:B:445:MET:HE2	1.96	0.48
1:A:282:LEU:HG	3:A:859:HOH:O	2.13	0.48
1:B:116:LYS:O	1:B:116:LYS:HG2	2.14	0.48
1:A:63:GLU:OE2	1:A:63:GLU:N	2.42	0.48
1:A:419:THR:HG21	1:A:526:THR:HG23	1.96	0.48
1:B:213:TRP:HZ2	1:B:217:ARG:NH1	2.11	0.48
1:B:473:THR:O	1:B:477:THR:HG23	2.13	0.48
1:B:202:ILE:HD11	1:B:210:LEU:HD22	1.96	0.47
1:A:342:VAL:O	1:A:343:SER:C	2.55	0.47
1:B:541:GLU:CD	1:B:541:GLU:H	2.23	0.47
1:A:267:GLN:HG2	1:A:274:LEU:HB2	1.96	0.47
1:B:529:VAL:O	1:B:533:LYS:HG3	2.15	0.47
1:A:210:LEU:HD23	1:A:238:THR:HG23	1.97	0.47
1:B:134:TRP:HB2	1:B:161:ASN:ND2	2.29	0.47
1:B:151:PRO:HB2	1:B:256:ARG:NH1	2.30	0.47
1:A:306:ALA:HA	1:A:310:GLU:OE1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:LYS:HE3	3:A:747:HOH:O	2.14	0.46
1:A:309:ALA:O	1:A:369:TYR:CE2	2.68	0.46
1:B:185:ARG:CZ	1:B:189:LEU:HD11	2.46	0.46
1:B:429:LEU:HD23	1:B:429:LEU:HA	1.60	0.46
1:A:407:ILE:CD1	1:A:525:GLN:HB3	2.45	0.46
1:B:440:PRO:HB2	1:B:443:GLU:OE2	2.15	0.46
1:A:153:LEU:HD12	1:A:153:LEU:C	2.41	0.46
1:A:351:GLU:OE2	1:A:375:LYS:NZ	2.39	0.46
1:B:447:CYS:O	1:B:447:CYS:SG	2.67	0.46
1:B:493:ASP:OD2	1:B:495:THR:OG1	2.33	0.45
1:B:449:GLU:HA	1:B:449:GLU:OE2	2.16	0.45
1:B:302:PRO:O	1:B:336:ARG:NH1	2.49	0.45
1:A:217:ARG:NH1	3:A:804:HOH:O	2.49	0.45
1:B:223:PRO:HD2	1:B:295:ASP:CB	2.47	0.45
1:B:582:LEU:HD23	1:B:582:LEU:HA	1.72	0.45
1:A:8:ALA:O	1:A:12:LYS:HE3	2.16	0.45
1:A:228:VAL:CA	1:A:231:THR:OG1	2.64	0.45
1:B:414:VAL:HG12	1:B:417:VAL:CG2	2.44	0.45
1:A:417:VAL:O	1:A:533:LYS:NZ	2.47	0.45
1:A:409:ARG:CD	3:A:847:HOH:O	2.65	0.44
1:B:308:PHE:HE2	1:B:332:GLU:HG3	1.83	0.44
1:B:408:VAL:O	1:B:409:ARG:C	2.60	0.44
1:A:399:GLU:OE2	1:A:431:LYS:HG2	2.18	0.44
1:B:399:GLU:O	1:B:403:GLN:HG3	2.17	0.44
1:A:293:GLU:CG	1:A:294:LYS:N	2.76	0.44
1:B:423:VAL:HG12	1:B:427:ARG:HD3	1.99	0.44
1:A:80:LEU:O	1:A:84:TYR:N	2.47	0.44
1:A:110:PRO:O	1:A:111:ASP:HB3	2.16	0.44
1:A:280:LYS:HB3	1:A:281:PRO:HD2	1.99	0.44
1:B:13:ASP:HB3	3:B:667:HOH:O	2.17	0.44
1:B:208:ARG:HG2	3:B:691:HOH:O	2.17	0.44
1:A:297:ILE:HG22	1:A:301:LEU:HD13	1.99	0.44
1:B:57:GLU:OE2	1:B:57:GLU:HA	2.17	0.43
1:A:219:SER:HB2	1:A:334:SER:HB2	2.00	0.43
1:A:264:CYS:SG	1:A:285:LYS:HD2	2.58	0.43
1:B:371:THR:O	1:B:373:PHE:N	2.51	0.43
1:A:161:ASN:ND2	3:A:769:HOH:O	2.50	0.43
1:A:369:TYR:C	1:A:369:TYR:CD2	2.97	0.43
1:A:452:LEU:HA	1:A:452:LEU:HD23	1.68	0.43
1:A:564:GLU:H	1:A:564:GLU:CD	2.27	0.43
1:B:386:LEU:HG	1:B:387:ILE:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:GLN:HG3	1:B:390:ASN:N	2.34	0.43
1:A:227:PHE:O	1:A:231:THR:OG1	2.27	0.43
1:A:511:ASP:O	1:A:512:ILE:C	2.60	0.43
1:A:36:PHE:O	1:A:40:VAL:HG23	2.18	0.43
1:A:157:ALA:O	1:A:160:TYR:HB3	2.18	0.43
1:A:412:ARG:HH11	1:A:412:ARG:HD2	1.68	0.43
1:B:326:LEU:HD21	1:B:353:GLU:HB2	2.01	0.43
1:B:371:THR:O	1:B:372:VAL:C	2.62	0.43
1:A:53:CYS:O	1:A:57:GLU:HG3	2.19	0.43
1:B:236:ASP:O	1:B:240:VAL:HG23	2.19	0.43
1:B:515:LEU:HA	1:B:516:PRO:HD2	1.88	0.43
1:A:112:LEU:HD23	1:A:112:LEU:HA	1.77	0.42
1:A:392:ASP:O	1:A:396:LYS:HB2	2.19	0.42
1:A:414:VAL:N	1:A:415:PRO:HD3	2.34	0.42
1:B:126:PHE:HZ	1:B:165:GLN:HG2	1.85	0.42
1:B:339:GLU:HG2	1:B:340:TYR:N	2.34	0.42
1:B:403:GLN:HG2	1:B:430:GLY:HA3	2.01	0.42
1:B:126:PHE:HZ	1:B:165:GLN:HG3	1.85	0.42
1:B:223:PRO:HB2	1:B:297:ILE:HA	2.01	0.42
1:B:414:VAL:CG1	1:B:417:VAL:CG2	2.95	0.42
1:B:539:THR:OG1	1:B:542:GLN:HG3	2.19	0.42
1:A:366:HIS:O	1:A:370:SER:HB3	2.20	0.42
1:B:167:CYS:C	1:B:169:GLN:H	2.26	0.42
1:B:213:TRP:CD1	3:B:659:HOH:O	2.71	0.42
1:B:385:ASN:ND2	1:B:385:ASN:N	2.66	0.42
1:B:137:TYR:O	1:B:138:LEU:C	2.63	0.42
1:B:377:LYS:O	1:B:381:ASP:OD2	2.37	0.42
1:B:511:ASP:OD2	1:B:512:ILE:N	2.53	0.42
1:A:153:LEU:HD13	1:A:153:LEU:HA	1.81	0.42
1:A:408:VAL:CG1	1:A:412:ARG:NH1	2.83	0.41
1:B:519:GLU:CG	3:B:722:HOH:O	2.42	0.41
1:A:66:LEU:O	1:A:70:PHE:HD2	2.03	0.41
1:A:131:LYS:O	1:A:134:TRP:HB3	2.19	0.41
1:A:425:VAL:O	1:A:429:LEU:HG	2.20	0.41
1:B:305:THR:HB	1:B:310:GLU:HG3	2.01	0.41
1:A:460:CYS:O	1:A:464:GLU:N	2.42	0.41
1:B:378:HIS:C	1:B:378:HIS:HD2	2.28	0.41
1:B:223:PRO:HB2	1:B:298:PRO:HD2	2.02	0.41
1:A:318:TYR:OH	1:A:357:GLU:OE2	2.33	0.41
1:A:328:SER:O	1:A:332:GLU:HG2	2.20	0.41
1:A:331:TYR:OH	1:A:335:ARG:CZ	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:TYR:HB3	1:A:184:MET:HE3	2.03	0.41
1:A:495:THR:CA	3:A:848:HOH:O	2.68	0.41
1:B:431:LYS:HB3	1:B:431:LYS:HE2	1.82	0.41
1:A:298:PRO:O	1:A:301:LEU:HD11	2.15	0.41
1:A:24:LEU:HB2	1:A:43:VAL:HG21	2.01	0.41
1:A:274:LEU:O	1:A:277:CYS:HB2	2.21	0.41
1:A:387:ILE:HD11	1:A:445:MET:HG2	2.03	0.41
1:B:330:LEU:CD1	1:B:349:ALA:HB2	2.46	0.41
1:B:464:GLU:O	1:B:464:GLU:OE2	2.38	0.41
1:A:112:LEU:HA	1:A:113:PRO:HD2	1.90	0.41
1:A:171:GLU:OE2	1:A:171:GLU:N	2.42	0.41
1:A:200:ALA:O	1:A:204:LYS:HB2	2.21	0.41
1:B:152:GLU:O	1:B:155:TYR:HB3	2.21	0.41
1:A:579:GLN:OE1	3:A:806:HOH:O	2.22	0.40
1:B:353:GLU:HG2	1:B:354:ALA:N	2.34	0.40
1:A:159:LYS:HA	1:A:159:LYS:HD3	1.81	0.40
1:B:267:GLN:CG	1:B:274:LEU:HB2	2.51	0.40
1:B:378:HIS:O	1:B:382:GLU:HG3	2.21	0.40
1:B:511:ASP:OD2	1:B:511:ASP:C	2.64	0.40
1:B:377:LYS:HD3	1:B:377:LYS:HA	1.77	0.40
1:A:437:CYS:HA	1:A:444:ARG:HD3	2.03	0.40
1:A:501:PHE:HB2	1:A:534:HIS:CE1	2.56	0.40
1:B:173:LYS:HB2	1:B:173:LYS:HE2	1.86	0.40
1:B:213:TRP:CZ2	1:B:217:ARG:HD2	2.57	0.40
1:B:223:PRO:CG	1:B:295:ASP:HB3	2.51	0.40
1:B:131:LYS:HD2	1:B:131:LYS:HA	1.80	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	584/583 (100%)	545 (93%)	38 (6%)	1 (0%)	43	61
1	B	583/583 (100%)	532 (91%)	51 (9%)	0	100	100
All	All	1167/1166 (100%)	1077 (92%)	89 (8%)	1 (0%)	48	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	ASP

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	524/521 (101%)	470 (90%)	54 (10%)	7	13
1	B	523/521 (100%)	471 (90%)	52 (10%)	7	14
All	All	1047/1042 (100%)	941 (90%)	106 (10%)	7	13

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

Mol	Chain	Res	Type
1	A	1	ASP
1	A	54	VAL
1	A	65[A]	SER
1	A	65[B]	SER
1	A	111	ASP
1	A	114	LYS
1	A	118	ASP
1	A	121	THR
1	A	127	LYS
1	A	131	LYS
1	A	139	TYR
1	A	153	LEU
1	A	165	GLN
1	A	181	ILE
1	A	188	VAL

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Mol	Chain	Res	Type
1	A	192	SER
1	A	202	ILE
1	A	204	LYS
1	A	224	LYS
1	A	231	THR
1	A	282	LEU
1	A	292	VAL
1	A	293	GLU
1	A	301	LEU
1	A	305	THR
1	A	310	GLU
1	A	312	LYS
1	A	316	LYS
1	A	358	GLU
1	A	374	ASP
1	A	377	LYS
1	A	379	LEU
1	A	380	VAL
1	A	381	ASP
1	A	383	PRO
1	A	385	ASN
1	A	407	ILE
1	A	409	ARG
1	A	438	THR
1	A	440	PRO
1	A	441	GLU
1	A	448	THR
1	A	450	ASP
1	A	458	ARG
1	A	464	GLU
1	A	469	SER
1	A	479	SER
1	A	509	HIS
1	A	517	ASP
1	A	520	LYS
1	A	532	LEU
1	A	540	GLU
1	A	541	GLU
1	A	563	LYS
1	B	2	THR
1	B	6	GLU
1	B	7	ILE

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Mol	Chain	Res	Type
1	B	54	VAL
1	B	58	SER
1	B	76	LYS
1	B	86	ASP
1	B	98	ARG
1	B	116	LYS
1	B	166	GLU
1	B	191	SER
1	B	208	ARG
1	B	214	SER
1	B	229	GLU
1	B	244	CYS
1	B	251	GLU
1	B	268	ASP
1	B	275	LYS
1	B	280	LYS
1	B	286	SER
1	B	291	GLU
1	B	299	GLU
1	B	320	GLU
1	B	326	LEU
1	B	336	ARG
1	B	339	GLU
1	B	343	SER
1	B	355	THR
1	B	359	CYS
1	B	364	ASP
1	B	370	SER
1	B	371	THR
1	B	374	ASP
1	B	375	LYS
1	B	378	HIS
1	B	379	LEU
1	B	385	ASN
1	B	386	LEU
1	B	387	ILE
1	B	389	GLN
1	B	392	ASP
1	B	396	LYS
1	B	407	ILE
1	B	431	LYS
1	B	447	CYS

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Mol	Chain	Res	Type
1	B	464	GLU
1	B	478	GLU
1	B	507	THR
1	B	512	ILE
1	B	561	ASP
1	B	564	GLU
1	B	569	VAL

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	18	HIS
1	A	39	HIS
1	A	59	HIS
1	A	220	GLN
1	A	317	ASN
1	A	319	GLN
1	A	337	HIS
1	A	366	HIS
1	A	384	GLN
1	A	482	ASN
1	A	509	HIS
1	B	161	ASN
1	B	165	GLN
1	B	267	GLN
1	B	319	GLN
1	B	337	HIS
1	B	378	HIS
1	B	385	ASN
1	B	393	GLN
1	B	482	ASN
1	B	549	ASN

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

1 ligand is 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	PGE	A	601	-	9,9,9	0.54	0	8,8,8	0.44	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	PGE	A	601	-	-	4/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	PGE	O2-C3-C4-O3
2	A	601	PGE	O1-C1-C2-O2
2	A	601	PGE	C3-C4-O3-C5
2	A	601	PGE	O3-C5-C6-O4

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	PGE	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	583/583 (100%)	-0.25	0 100 100	39, 68, 96, 118	3 (0%)
1	B	583/583 (100%)	-0.14	1 (0%) 91 90	41, 74, 107, 127	2 (0%)
All	All	1166/1166 (100%)	-0.20	1 (0%) 92 91	39, 71, 102, 127	5 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	487	PHE	2.3

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(Å ²)	Q<0.9
2	PGE	A	601	10/10	0.90	0.09	61,65,66,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.