



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:48 PM UTC

PDB ID : 4EMX / pdb_00004emx
Title : Crystal structure analysis of Human Serum Albumin in complex with chloride anions at cryogenic temperature
Authors : Botti, H.; Bonilla, L.; Trajtenberg, F.; Radi, R.; Buschiazzi, A.
Deposited on : 2012-04-12
Resolution : 2.30 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
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

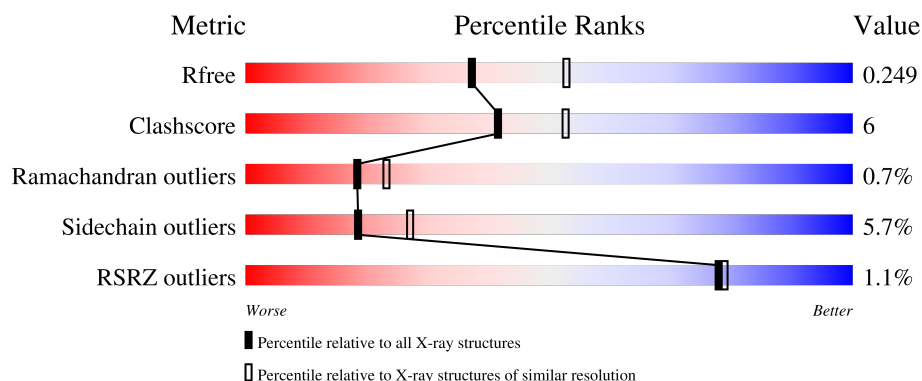
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	% 79% 18% ..
1	B	585	% 79% 18% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9377 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	581	Total	C	N	O	S	0	5	0
			4600	2903	784	872	41			
1	B	579	Total	C	N	O	S	0	4	0
			4543	2867	772	863	41			

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Cl	0	0
			3	3		
2	B	3	Total	Cl	0	0
			3	3		

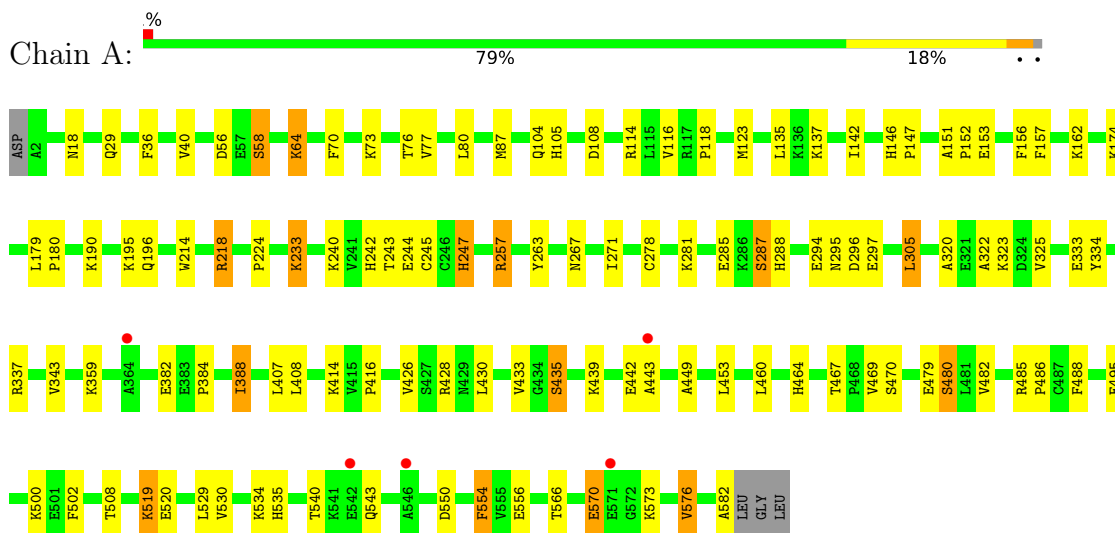
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	123	Total	O	0	0
			123	123		
3	B	105	Total	O	0	0
			105	105		

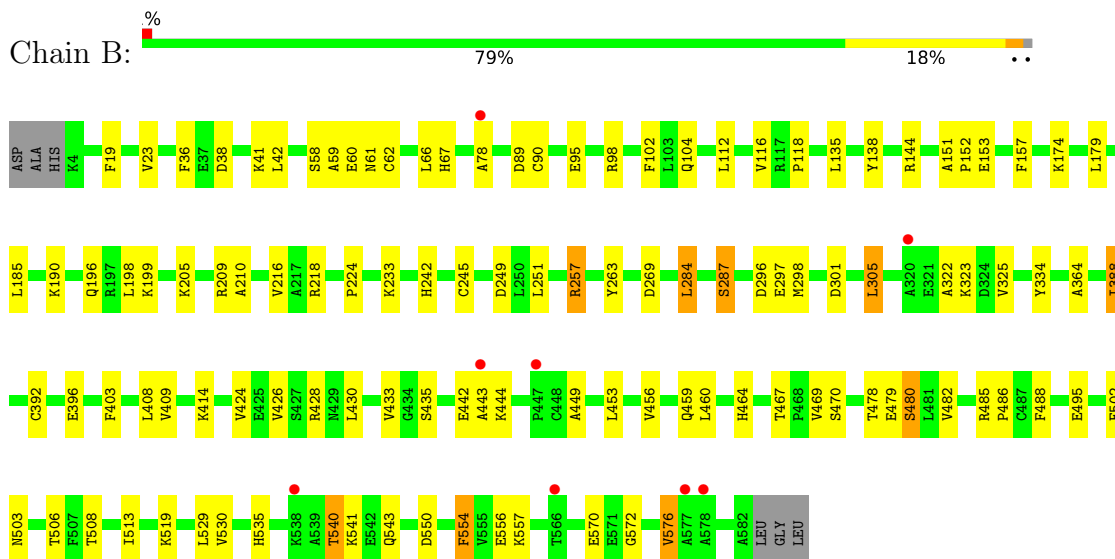
3 Residue-property plots

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	58.88Å 59.23Å 95.61Å 75.17° 87.83° 74.20°	Depositor
Resolution (Å)	25.50 – 2.30 25.50 – 2.30	Depositor EDS
% Data completeness (in resolution range)	93.0 (25.50-2.30) 93.0 (25.50-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 2.31Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.187 , 0.238 0.192 , 0.249	Depositor DCC
R_{free} test set	1009 reflections (2.03%)	wwPDB-VP
Wilson B-factor (Å ²)	44.8	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 54.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9377	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.43% 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: CL

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	1.06	7/4698 (0.1%)	1.15	5/6344 (0.1%)
1	B	1.01	2/4639 (0.0%)	1.15	12/6270 (0.2%)
All	All	1.03	9/9337 (0.1%)	1.15	17/12614 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	102	PHE	N-CA	6.42	1.54	1.46
1	A	146	HIS	CG-CD2	6.03	1.42	1.35
1	A	242	HIS	ND1-CE1	5.51	1.38	1.32
1	A	242	HIS	CG-CD2	5.41	1.41	1.35
1	A	247[A]	HIS	CG-CD2	5.26	1.41	1.35
1	A	247[B]	HIS	CG-CD2	5.26	1.41	1.35
1	A	146	HIS	ND1-CE1	5.22	1.37	1.32
1	A	18	ASN	CA-C	5.18	1.59	1.52
1	B	242	HIS	ND1-CE1	5.10	1.37	1.32

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	179	LEU	CA-C-N	-8.00	111.56	119.64
1	B	179	LEU	C-N-CA	-8.00	111.56	119.64
1	B	89	ASP	N-CA-C	-6.49	103.33	111.11
1	B	36	PHE	N-CA-C	5.98	117.80	111.28
1	B	444	LYS	N-CA-C	-5.76	106.04	114.39
1	B	198	LEU	N-CA-C	-5.74	105.10	111.36
1	A	108	ASP	CA-C-N	-5.66	116.20	123.16
1	A	108	ASP	C-N-CA	-5.66	116.20	123.16
1	B	409	VAL	N-CA-C	-5.65	105.02	110.72
1	B	456	VAL	N-CA-C	5.64	116.37	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	216	VAL	N-CA-CB	5.47	116.96	110.55
1	A	257	ARG	CB-CG-CD	-5.37	98.94	111.30
1	B	403	PHE	N-CA-C	-5.20	105.30	111.69
1	A	382	GLU	N-CA-C	5.18	116.73	111.14
1	B	78	ALA	N-CA-C	5.07	117.54	111.71
1	B	257	ARG	CB-CG-CD	-5.07	99.64	111.30
1	A	142	ILE	CB-CA-C	-5.01	105.31	112.22

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	4600	0	4487	68	0
1	B	4543	0	4408	58	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	123	0	0	5	0
3	B	105	0	0	5	0
All	All	9377	0	8895	116	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 6.

All (116) 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:500:LYS:NZ	3:A:779:HOH:O	2.04	0.88
1:A:464:HIS:HE1	1:A:470:SER:H	1.22	0.84
1:B:464:HIS:HE1	1:B:470:SER:H	1.27	0.81
1:A:320:ALA:HA	1:B:364:ALA:HB1	1.63	0.79
1:A:104:GLN:HG2	3:A:753:HOH:O	1.84	0.78
1:B:430:LEU:O	1:B:433:VAL:HG12	1.84	0.77
1:A:156:PHE:HE1	1:A:285:GLU:HG2	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:LEU:HD22	3:B:766:HOH:O	1.89	0.71
1:B:112:LEU:HD11	1:B:144:ARG:NH2	2.06	0.70
1:B:464:HIS:CE1	1:B:470:SER:H	2.08	0.70
1:A:305:LEU:HD22	1:A:334:TYR:HD2	1.56	0.69
1:A:320:ALA:HA	1:B:364:ALA:CB	2.23	0.69
1:A:64:LYS:HZ1	1:B:104:GLN:NE2	1.90	0.68
1:A:156:PHE:CE1	1:A:285:GLU:HG2	2.27	0.68
1:B:67:HIS:CE1	1:B:249:ASP:OD1	2.47	0.68
1:B:224:PRO:HD2	1:B:296:ASP:HB3	1.78	0.65
1:A:56:ASP:OD1	1:A:58:SER:HB2	1.97	0.64
1:A:464:HIS:CE1	1:A:470:SER:H	2.11	0.63
1:B:305:LEU:HD22	1:B:334:TYR:HD2	1.63	0.63
1:A:479:GLU:O	1:A:480:SER:HB2	1.99	0.63
1:A:64:LYS:NZ	1:B:104:GLN:NE2	2.46	0.63
1:B:151:ALA:HB3	1:B:152:PRO:CD	2.30	0.62
1:A:479:GLU:O	1:A:480:SER:CB	2.48	0.62
1:B:90:CYS:O	1:B:98:ARG:HG3	2.01	0.61
1:A:64:LYS:HZ1	1:B:104:GLN:HE22	1.49	0.60
1:A:414:LYS:HE3	1:A:488:PHE:O	2.02	0.59
1:A:87:MET:HE1	1:A:105:HIS:HB3	1.84	0.58
1:A:243:THR:O	1:A:247[B]:HIS:HD2	1.87	0.57
1:B:479:GLU:O	1:B:480:SER:CB	2.52	0.57
1:A:29:GLN:HG2	1:A:147:PRO:HA	1.88	0.56
1:B:459:GLN:NE2	3:B:772:HOH:O	2.34	0.56
1:A:118:PRO:HD2	1:A:123:MET:HE3	1.88	0.55
1:A:243:THR:O	1:A:247[B]:HIS:CD2	2.60	0.55
1:A:257:ARG:CZ	1:A:287:SER:HB3	2.36	0.55
1:A:464:HIS:CE1	1:A:469:VAL:H	2.24	0.55
1:B:257:ARG:CZ	1:B:287:SER:HB3	2.37	0.54
1:B:414:LYS:HE3	1:B:488:PHE:O	2.08	0.54
1:A:224:PRO:HD2	1:A:296:ASP:HB3	1.90	0.53
1:A:278:CYS:O	1:A:281[A]:LYS:HG3	2.08	0.53
1:B:67:HIS:HE1	1:B:249:ASP:OD1	1.90	0.52
1:A:485:ARG:HB3	1:A:486:PRO:HD3	1.90	0.52
1:A:502:PHE:HB2	1:A:535:HIS:CE1	2.44	0.52
1:B:153:GLU:HG3	1:B:157:PHE:HE1	1.74	0.52
1:A:430:LEU:O	1:A:433:VAL:HG12	2.10	0.52
1:B:424:VAL:O	1:B:428:ARG:HG3	2.10	0.51
1:A:408:LEU:HD22	1:A:529:LEU:HD23	1.92	0.50
1:A:573:LYS:HA	1:A:576:VAL:HG13	1.93	0.50
1:B:550:ASP:O	1:B:554:PHE:HB3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:MET:CE	1:A:105:HIS:HB3	2.41	0.50
1:A:257:ARG:NH2	3:A:823:HOH:O	2.35	0.49
1:B:449:ALA:O	1:B:453:LEU:HG	2.13	0.49
1:A:153:GLU:OE2	1:A:288:HIS:ND1	2.39	0.48
1:A:322:ALA:HB1	1:A:325:VAL:HB	1.95	0.48
1:A:135:LEU:HD11	1:A:162:LYS:HB2	1.95	0.48
1:A:550:ASP:O	1:A:554:PHE:HB3	2.12	0.48
1:B:19:PHE:O	1:B:23:VAL:HG23	2.13	0.48
1:B:269[B]:ASP:N	1:B:269[B]:ASP:OD1	2.47	0.47
1:B:408:LEU:HD22	1:B:529:LEU:HD23	1.95	0.47
1:B:205:LYS:HD3	3:B:804:HOH:O	2.16	0.46
1:A:408:LEU:HD21	1:A:530:VAL:CG2	2.46	0.46
1:B:502:PHE:HB2	1:B:535:HIS:CE1	2.50	0.46
1:A:543:GLN:NE2	1:A:582:ALA:O	2.48	0.46
1:B:540:THR:O	1:B:543:GLN:N	2.49	0.46
1:A:320:ALA:CA	1:B:364:ALA:HB1	2.39	0.46
1:B:66:LEU:HD13	1:B:251:LEU:HD12	1.97	0.46
1:A:384:PRO:O	1:A:388:ILE:HG12	2.16	0.45
1:B:190:LYS:HB3	1:B:190:LYS:HE2	1.73	0.45
1:B:60:GLU:O	1:B:61[B]:ASN:HB2	2.16	0.45
1:B:153:GLU:HG3	1:B:157:PHE:CE1	2.52	0.45
1:B:388:ILE:HD13	1:B:388:ILE:N	2.32	0.45
1:A:320:ALA:C	1:B:364:ALA:CB	2.89	0.45
1:B:392:CYS:O	1:B:396:GLU:HG2	2.17	0.45
1:B:151:ALA:HB3	1:B:152:PRO:HD3	1.98	0.45
1:A:190:LYS:HB3	1:A:190:LYS:HE2	1.69	0.45
1:B:572:GLY:O	1:B:576:VAL:HG23	2.17	0.45
1:B:116:VAL:O	1:B:118:PRO:HD3	2.18	0.44
1:A:233:LYS:HE3	1:A:263:TYR:CZ	2.52	0.44
1:A:240:LYS:O	1:A:244:GLU:HG3	2.16	0.44
1:A:428:ARG:HH12	1:A:519:LYS:NZ	2.16	0.44
1:A:73:LYS:HA	1:A:73:LYS:HD3	1.89	0.44
1:A:196:GLN:NE2	1:A:196:GLN:HA	2.32	0.44
1:B:209:ARG:HB3	3:B:734:HOH:O	2.17	0.44
1:A:179:LEU:N	1:A:180:PRO:CD	2.80	0.44
1:A:267:ASN:O	1:A:271:ILE:HG13	2.18	0.43
1:A:195:LYS:NZ	3:A:782:HOH:O	2.51	0.43
1:A:408:LEU:HD21	1:A:530:VAL:HG23	1.99	0.43
1:B:59:ALA:HB3	1:B:62:CYS:SG	2.58	0.43
1:A:214:TRP:CD1	1:A:343:VAL:HG11	2.53	0.43
1:A:76:THR:HA	1:B:95:GLU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:MET:HE3	1:B:298:MET:HB2	1.83	0.43
1:A:218:ARG:NH2	1:A:295:ASN:OD1	2.49	0.43
1:A:36:PHE:O	1:A:40:VAL:HG23	2.18	0.43
1:B:210:ALA:N	3:B:734:HOH:O	2.50	0.43
1:A:320:ALA:CA	1:B:364:ALA:CB	2.93	0.43
1:B:196:GLN:O	1:B:199:LYS:N	2.51	0.43
1:B:322:ALA:HB1	1:B:325:VAL:HB	2.00	0.43
1:B:464:HIS:CE1	1:B:469:VAL:H	2.36	0.43
1:B:233:LYS:HE3	1:B:263:TYR:CE2	2.55	0.42
1:A:426:VAL:HG21	1:A:460:LEU:HB2	2.00	0.42
1:A:320:ALA:C	1:B:364:ALA:HB2	2.45	0.42
1:A:196:GLN:NE2	3:A:773:HOH:O	2.52	0.42
1:A:153:GLU:O	1:A:157:PHE:HD1	2.02	0.42
1:A:114:ARG:NH1	1:A:520:GLU:HG2	2.34	0.42
1:B:408:LEU:HD21	1:B:530:VAL:HG23	2.01	0.42
1:A:70:PHE:N	1:A:70:PHE:CD1	2.87	0.42
1:A:333:GLU:HB3	1:A:337:ARG:NH1	2.34	0.42
1:A:416:PRO:O	1:A:534:LYS:HE2	2.19	0.42
1:A:407:LEU:HD13	1:A:430:LEU:HB3	2.02	0.42
1:A:435:SER:O	1:A:439:LYS:HE3	2.20	0.41
1:B:135:LEU:O	1:B:138:TYR:HB3	2.21	0.41
1:B:426:VAL:HG21	1:B:460:LEU:HB2	2.03	0.41
1:B:503:ASN:HB3	1:B:506:THR:HB	2.03	0.41
1:A:151:ALA:N	1:A:152:PRO:HD2	2.36	0.40
1:B:38:ASP:O	1:B:42:LEU:HG	2.21	0.40
1:A:449:ALA:O	1:A:453:LEU:HG	2.22	0.40
1:B:485:ARG:HB3	1:B:486:PRO:HD3	2.03	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	584/585 (100%)	562 (96%)	18 (3%)	4 (1%)	18	23
1	B	581/585 (99%)	555 (96%)	22 (4%)	4 (1%)	18	23
All	All	1165/1170 (100%)	1117 (96%)	40 (3%)	8 (1%)	18	23

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	443	ALA
1	A	480	SER
1	B	443	ALA
1	B	480	SER
1	A	442	GLU
1	B	442	GLU
1	B	576	VAL
1	A	570	GLU

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	497/511 (97%)	468 (94%)	29 (6%)	18	26
1	B	488/511 (96%)	461 (94%)	27 (6%)	19	28
All	All	985/1022 (96%)	929 (94%)	56 (6%)	18	27

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	SER
1	A	64	LYS
1	A	77	VAL
1	A	80	LEU
1	A	116	VAL
1	A	137	LYS
1	A	174	LYS
1	A	218	ARG

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Mol	Chain	Res	Type
1	A	233	LYS
1	A	245	CYS
1	A	287	SER
1	A	294	GLU
1	A	297	GLU
1	A	305	LEU
1	A	323	LYS
1	A	359	LYS
1	A	388	ILE
1	A	435	SER
1	A	467	THR
1	A	482	VAL
1	A	495	GLU
1	A	508	THR
1	A	519	LYS
1	A	540	THR
1	A	554	PHE
1	A	556	GLU
1	A	566	THR
1	A	570	GLU
1	A	576	VAL
1	B	41	LYS
1	B	58	SER
1	B	174	LYS
1	B	185	LEU
1	B	218	ARG
1	B	245	CYS
1	B	284	LEU
1	B	287	SER
1	B	297	GLU
1	B	301	ASP
1	B	305	LEU
1	B	323	LYS
1	B	388	ILE
1	B	435	SER
1	B	467	THR
1	B	478	THR
1	B	482	VAL
1	B	495	GLU
1	B	508	THR
1	B	513	ILE
1	B	519	LYS

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Mol	Chain	Res	Type
1	B	540	THR
1	B	541	LYS
1	B	554	PHE
1	B	556	GLU
1	B	557	LYS
1	B	570	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	A	196	GLN
1	A	204	GLN
1	A	221	GLN
1	A	267	ASN
1	A	367	HIS
1	A	464	HIS
1	A	483	ASN
1	B	33	GLN
1	B	67	HIS
1	B	104	GLN
1	B	109	ASN
1	B	196	GLN
1	B	247	HIS
1	B	267	ASN
1	B	464	HIS
1	B	483	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

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	581/585 (99%)	-0.03	5 (0%) 81 82	25, 69, 129, 178	5 (0%)
1	B	579/585 (98%)	0.04	8 (1%) 73 75	32, 72, 129, 173	4 (0%)
All	All	1160/1170 (99%)	0.01	13 (1%) 78 79	25, 71, 129, 178	9 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	578	ALA	2.9
1	B	566	THR	2.8
1	A	443	ALA	2.7
1	B	320	ALA	2.7
1	B	78	ALA	2.5
1	A	546	ALA	2.4
1	B	443	ALA	2.4
1	B	577	ALA	2.3
1	A	542	GLU	2.3
1	A	571	GLU	2.2
1	A	364	ALA	2.1
1	B	447	PRO	2.1
1	B	538	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no 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	CL	B	602	1/1	0.92	0.11	81,81,81,81	0
2	CL	A	603	1/1	0.93	0.13	92,92,92,92	0
2	CL	A	601	1/1	0.93	0.11	98,98,98,98	0
2	CL	B	601	1/1	0.94	0.11	80,80,80,80	0
2	CL	B	603	1/1	0.96	0.06	78,78,78,78	0
2	CL	A	602	1/1	0.98	0.11	67,67,67,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.