



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 24, 2026 – 09:17 PM EDT

PDB ID : 1AO6 / pdb_00001ao6
Title : CRYSTAL STRUCTURE OF HUMAN SERUM ALBUMIN
Authors : Sugio, S.; Mochizuki, S.; Noda, M.; Kashima, A.
Deposited on : 1997-07-18
Resolution : 2.50 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

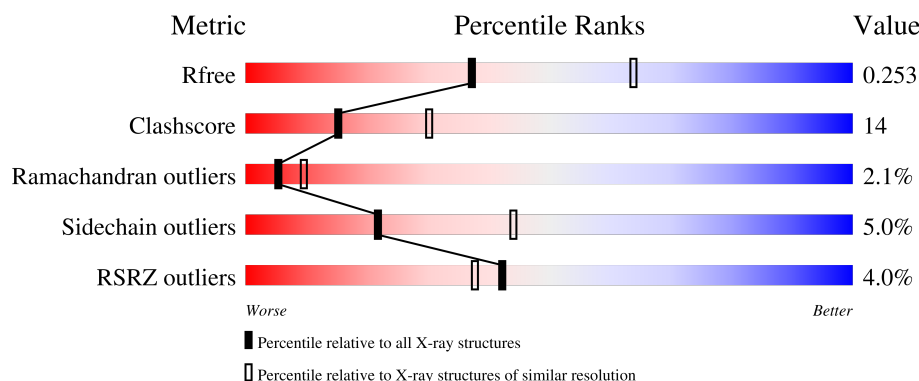
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	4% 61% 32% 6%
1	B	585	4% 64% 30%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9205 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
			4599	2903	776	879	41			
1	B	578	Total	C	N	O	S	0	0	0
			4599	2903	776	879	41			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	O	0	0
			3	3		
2	B	4	Total	O	0	0
			4	4		

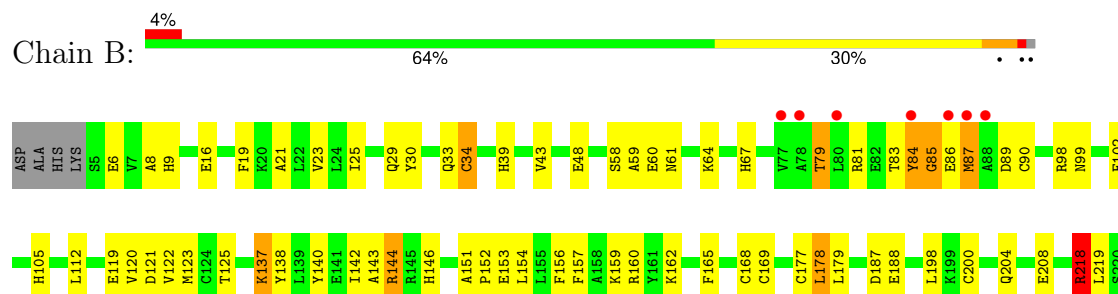
3 Residue-property plots

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	59.68Å 96.98Å 59.72Å 91.07° 103.50° 75.08°	Depositor
Resolution (Å)	50.00 – 2.50 50.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	86.2 (50.00-2.50) 86.2 (50.00-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 2.51Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.218 , 0.282 0.195 , 0.253	Depositor DCC
R_{free} test set	3814 reflections (10.18%)	wwPDB-VP
Wilson B-factor (Å ²)	42.9	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 67.4	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	9205	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.52% 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

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	0.80	2/4688 (0.0%)	1.24	46/6324 (0.7%)
1	B	0.83	1/4688 (0.0%)	1.22	40/6324 (0.6%)
All	All	0.82	3/9376 (0.0%)	1.23	86/12648 (0.7%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	87	MET	SD-CE	6.57	1.96	1.79
1	A	87	MET	SD-CE	5.35	1.93	1.79
1	A	25	ILE	CA-CB	5.31	1.61	1.54

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	204	GLN	N-CA-C	9.26	121.38	111.28
1	A	207	GLY	N-CA-C	8.63	120.15	111.95
1	A	178	LEU	N-CA-C	8.06	119.84	111.14
1	A	86	GLU	N-CA-C	8.04	122.04	111.75
1	B	479	GLU	N-CA-C	7.95	120.85	111.71
1	B	445	ARG	N-CA-C	7.87	121.00	111.40
1	B	307	ALA	N-CA-C	7.87	119.86	111.28
1	A	92	ALA	N-CA-C	-7.80	103.90	113.41
1	A	415	VAL	CA-C-N	7.57	127.28	119.56
1	A	415	VAL	C-N-CA	7.57	127.28	119.56
1	A	70	PHE	N-CA-C	7.35	119.29	111.28
1	A	479	GLU	N-CA-C	7.16	119.08	111.28
1	A	168	CYS	N-CA-C	7.07	121.52	112.34
1	A	497	TYR	N-CA-C	7.01	120.54	110.10
1	A	339	PRO	N-CA-C	-6.99	105.61	114.35
1	B	522	GLN	N-CA-C	-6.89	103.84	111.36
1	A	34	CYS	CA-C-N	6.80	126.83	119.90
1	A	34	CYS	C-N-CA	6.80	126.83	119.90
1	B	86	GLU	N-CA-C	6.75	120.39	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	445	ARG	N-CA-C	6.44	118.87	111.02
1	B	339	PRO	N-CA-C	-6.44	106.31	114.35
1	A	257	ARG	N-CA-C	-6.39	104.41	111.82
1	A	399	GLY	N-CA-C	-6.38	103.63	112.18
1	A	23	VAL	N-CA-C	-6.38	104.53	110.53
1	A	398	LEU	N-CA-C	6.37	118.30	111.36
1	B	458	ASN	N-CA-C	-6.36	104.35	111.28
1	B	261	ALA	N-CA-C	-6.36	104.35	111.28
1	A	342	SER	N-CA-C	-6.33	101.57	110.50
1	B	399	GLY	N-CA-C	-6.29	104.75	112.68
1	B	375	ASP	N-CA-C	-6.28	105.75	113.41
1	A	84	TYR	N-CA-C	6.28	118.91	110.88
1	B	365	ASP	CA-C-N	6.26	127.66	119.84
1	B	365	ASP	C-N-CA	6.26	127.66	119.84
1	A	381	VAL	N-CA-C	6.17	116.95	110.72
1	B	16	GLU	N-CA-C	6.17	118.80	111.33
1	B	48	GLU	N-CA-C	-6.16	103.51	111.02
1	B	360	CYS	N-CA-C	6.11	118.02	111.36
1	B	125	THR	N-CA-C	-6.07	104.58	111.14
1	A	456	VAL	CB-CA-C	-6.05	104.11	112.04
1	A	571	GLU	N-CA-C	-6.05	104.77	111.36
1	B	179	LEU	N-CA-C	6.00	121.06	113.25
1	B	497	TYR	N-CA-C	5.99	119.04	110.24
1	A	146	HIS	CA-C-N	5.97	125.65	119.56
1	A	146	HIS	C-N-CA	5.97	125.65	119.56
1	B	469	VAL	CB-CA-C	-5.93	105.78	111.05
1	A	250	LEU	N-CA-C	5.91	118.96	111.69
1	B	146	HIS	CA-C-N	5.85	125.55	119.82
1	B	146	HIS	C-N-CA	5.85	125.55	119.82
1	A	437	CYS	N-CA-C	5.79	121.00	113.88
1	A	275	LEU	N-CA-C	5.79	118.81	111.69
1	B	542	GLU	N-CA-C	-5.68	105.23	111.82
1	A	498	VAL	CA-C-N	5.63	125.94	119.92
1	A	498	VAL	C-N-CA	5.63	125.94	119.92
1	B	478	THR	N-CA-C	5.60	117.46	111.36
1	A	123	MET	N-CA-C	5.59	117.37	111.28
1	A	352	THR	N-CA-C	-5.55	104.92	110.97
1	A	133	THR	N-CA-C	-5.53	105.25	111.28
1	A	320	ALA	N-CA-C	5.53	116.98	111.07
1	B	84	TYR	N-CA-C	5.52	117.07	110.44
1	B	462	VAL	N-CA-C	5.49	117.91	111.05
1	B	218	ARG	N-CA-C	5.49	116.94	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	143	ALA	N-CA-C	5.49	117.26	111.28
1	B	8	ALA	N-CA-C	-5.46	105.41	111.36
1	A	459	GLN	N-CA-C	-5.43	105.44	111.36
1	A	19	PHE	N-CA-C	-5.38	105.11	110.97
1	B	506	THR	N-CA-C	5.38	119.53	112.92
1	A	375	ASP	N-CA-C	-5.37	105.09	111.69
1	A	368	GLU	N-CA-C	5.34	118.96	112.23
1	A	283	LEU	N-CA-C	5.34	120.12	111.37
1	A	32	GLN	N-CA-C	5.33	118.00	111.82
1	B	243	THR	N-CA-C	-5.32	105.48	111.28
1	B	178	LEU	N-CA-C	5.31	117.49	111.02
1	A	77	VAL	N-CA-C	5.27	118.21	113.10
1	B	570	GLU	N-CA-C	5.25	117.91	111.82
1	A	462	VAL	N-CA-C	5.25	115.97	110.62
1	B	437	CYS	N-CA-C	5.21	121.17	114.56
1	B	350	ALA	N-CA-C	-5.19	105.52	111.07
1	B	459	GLN	N-CA-C	-5.15	104.74	111.02
1	B	564	LYS	N-CA-C	-5.13	103.96	111.30
1	A	54	VAL	N-CA-C	-5.13	105.54	110.72
1	B	325	VAL	N-CA-C	-5.13	105.41	111.00
1	B	159	LYS	N-CA-C	-5.12	105.16	111.40
1	A	542	GLU	N-CA-C	-5.12	105.83	111.71
1	A	325	VAL	N-CA-C	-5.07	105.48	111.00
1	B	279	CYS	N-CA-C	5.06	118.94	112.87
1	B	162	LYS	N-CA-C	-5.01	105.29	111.40

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	4599	0	4518	135	0
1	B	4599	0	4518	112	0
2	A	3	0	0	0	0
2	B	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9205	0	9036	247	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 14.

All (247) 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:87:MET:HE1	1:B:105:HIS:HB3	1.20	1.18
1:A:87:MET:HE1	1:A:105:HIS:HB3	1.21	1.16
1:B:87:MET:CE	1:B:105:HIS:HB3	1.93	0.99
1:B:240:LYS:O	1:B:244:GLU:HG3	1.67	0.94
1:B:87:MET:HE1	1:B:105:HIS:CB	2.07	0.83
1:A:87:MET:CE	1:A:105:HIS:HB3	2.05	0.82
1:A:424:VAL:O	1:A:428:ARG:HG3	1.79	0.81
1:A:464:HIS:HE1	1:A:470:SER:H	1.28	0.81
1:B:307:ALA:HA	1:B:311:GLU:HB2	1.62	0.81
1:A:240:LYS:O	1:A:244:GLU:HG3	1.83	0.77
1:A:331:LEU:HD13	1:A:350:ALA:HB2	1.66	0.77
1:B:437:CYS:HA	1:B:440:HIS:HD2	1.50	0.76
1:B:119:GLU:HB2	1:B:122:VAL:HG23	1.68	0.75
1:B:384:PRO:O	1:B:388:ILE:HG12	1.86	0.75
1:A:356:THR:HG21	1:A:373:VAL:HG22	1.69	0.75
1:B:112:LEU:HD22	1:B:144:ARG:HH21	1.52	0.74
1:B:39:HIS:O	1:B:43:VAL:HG23	1.88	0.73
1:A:372:LYS:O	1:A:375:ASP:HB2	1.90	0.72
1:B:571:GLU:O	1:B:575:LEU:HG	1.89	0.71
1:A:464:HIS:CE1	1:A:470:SER:H	2.09	0.70
1:A:159:LYS:HD2	1:A:284:LEU:HD12	1.74	0.67
1:B:90:CYS:O	1:B:98:ARG:HG3	1.94	0.67
1:A:279:CYS:HA	1:A:286:LYS:HD3	1.77	0.67
1:B:509:PHE:HB2	1:B:568:PHE:HE1	1.60	0.66
1:A:437:CYS:HA	1:A:440:HIS:HD2	1.60	0.66
1:A:384:PRO:O	1:A:388:ILE:HG12	1.96	0.65
1:A:299:PRO:HB2	1:A:302:LEU:HG	1.77	0.65
1:A:440:HIS:ND1	1:A:444:LYS:HE3	2.11	0.65
1:A:442:GLU:HA	1:A:445:ARG:HD2	1.77	0.64
1:A:36:PHE:O	1:A:40:VAL:HG23	1.97	0.64
1:A:370:TYR:O	1:A:373:VAL:HG23	1.97	0.64
1:B:21:ALA:O	1:B:25:ILE:HG13	1.98	0.64
1:B:33:GLN:HB2	1:B:84:TYR:CD1	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:GLU:O	1:A:575:LEU:HG	1.98	0.64
1:B:415:VAL:O	1:B:418:VAL:HG23	1.98	0.64
1:A:377:PHE:O	1:A:381:VAL:HG23	1.98	0.64
1:B:218:ARG:HH21	1:B:221:GLN:HB2	1.64	0.63
1:A:417:GLN:HB3	1:A:469:VAL:HG12	1.80	0.63
1:B:383:GLU:HB3	1:B:384:PRO:HD3	1.81	0.61
1:A:112:LEU:HD22	1:A:144:ARG:NH2	2.15	0.61
1:A:552:ALA:O	1:A:556:GLU:HG2	2.00	0.61
1:A:151:ALA:HB3	1:A:152:PRO:HD3	1.80	0.61
1:A:141:GLU:O	1:A:145:ARG:HG3	2.01	0.61
1:A:25:ILE:O	1:A:29:GLN:HG3	2.00	0.60
1:A:156:PHE:HE1	1:A:285:GLU:HG3	1.65	0.60
1:A:81:ARG:HB2	1:A:85:GLY:HA2	1.84	0.60
1:A:237:ASP:O	1:A:241:VAL:HG23	2.01	0.60
1:A:25:ILE:HD13	1:A:154:LEU:HD23	1.84	0.59
1:B:548:MET:HE3	1:B:548:MET:HA	1.83	0.59
1:A:551:PHE:HA	1:A:554:PHE:HB3	1.84	0.59
1:A:151:ALA:HB2	1:A:250:LEU:HD13	1.84	0.59
1:A:414:LYS:C	1:A:416:PRO:HD3	2.27	0.59
1:A:516:LEU:O	1:A:521:ARG:NH2	2.36	0.59
1:B:34:CYS:HA	1:B:84:TYR:OH	2.02	0.59
1:B:151:ALA:HB3	1:B:152:PRO:HD3	1.84	0.58
1:A:307:ALA:HA	1:A:311:GLU:HB2	1.84	0.58
1:B:123:MET:HB3	1:B:165:PHE:HE2	1.69	0.58
1:B:540:THR:HG22	1:B:544:LEU:HG	1.85	0.58
1:B:224:PRO:HD2	1:B:296:ASP:HB3	1.85	0.58
1:B:153:GLU:O	1:B:157:PHE:HD1	1.86	0.58
1:A:485:ARG:HB3	1:A:486:PRO:HD3	1.86	0.57
1:B:262:LYS:C	1:B:262:LYS:HD2	2.29	0.57
1:A:498:VAL:HG13	1:A:498:VAL:O	2.05	0.57
1:A:449:ALA:O	1:A:453:LEU:HG	2.04	0.57
1:B:506:THR:HG22	1:B:506:THR:O	2.05	0.57
1:A:276:LYS:HD2	1:A:277:GLU:HG3	1.88	0.56
1:B:112:LEU:CD2	1:B:144:ARG:HH21	2.19	0.56
1:B:551:PHE:O	1:B:555:VAL:HG23	2.05	0.56
1:A:103:LEU:HD11	1:A:247:HIS:CD2	2.41	0.56
1:B:259:ASP:O	1:B:262:LYS:HB3	2.05	0.56
1:B:356:THR:HG21	1:B:373:VAL:HG22	1.87	0.56
1:B:424:VAL:O	1:B:428:ARG:HG3	2.05	0.56
1:B:299:PRO:HB2	1:B:302:LEU:HG	1.88	0.55
1:A:408:LEU:HD23	1:A:427:SER:CB	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:PRO:O	1:A:443:ALA:N	2.40	0.55
1:A:145:ARG:HG3	1:A:145:ARG:HH11	1.72	0.55
1:A:540:THR:HG22	1:A:544:LEU:HG	1.88	0.55
1:B:156:PHE:CE1	1:B:285:GLU:HG3	2.41	0.55
1:B:319:TYR:CE1	1:B:323:LYS:HB2	2.42	0.54
1:A:120:VAL:HG21	1:A:175:ALA:HA	1.88	0.54
1:A:196:GLN:NE2	1:A:196:GLN:HA	2.22	0.54
1:A:5:SER:HA	1:A:62:CYS:O	2.08	0.54
1:B:83:THR:HG22	1:B:84:TYR:CE1	2.43	0.54
1:B:156:PHE:HE1	1:B:285:GLU:HG3	1.73	0.54
1:B:112:LEU:HD22	1:B:144:ARG:NH2	2.21	0.54
1:B:319:TYR:O	1:B:323:LYS:HB3	2.07	0.53
1:B:441:PRO:O	1:B:443:ALA:N	2.41	0.53
1:B:138:TYR:O	1:B:142:ILE:HG12	2.08	0.53
1:A:383:GLU:HB3	1:A:384:PRO:HD3	1.91	0.53
1:A:387:LEU:HD22	1:A:485:ARG:NH1	2.24	0.53
1:A:103:LEU:HD11	1:A:247:HIS:HD2	1.73	0.53
1:A:378:LYS:HB2	1:A:379:PRO:HD3	1.90	0.52
1:B:119:GLU:HB2	1:B:122:VAL:CG2	2.38	0.52
1:A:319:TYR:CE1	1:A:323:LYS:HB2	2.45	0.52
1:B:225:LYS:HG2	1:B:299:PRO:HG3	1.91	0.52
1:A:439:LYS:HG3	1:A:439:LYS:O	2.10	0.51
1:B:25:ILE:O	1:B:29:GLN:HG3	2.09	0.51
1:A:415:VAL:N	1:A:416:PRO:HD3	2.24	0.51
1:B:464:HIS:HE1	1:B:470:SER:H	1.59	0.51
1:A:305:LEU:HD21	1:A:333:GLU:HB3	1.91	0.51
1:A:510:HIS:O	1:A:513:ILE:HG22	2.10	0.51
1:A:440:HIS:HB3	1:A:444:LYS:HB2	1.92	0.51
1:B:370:TYR:O	1:B:373:VAL:HG23	2.10	0.51
1:B:34:CYS:HB3	1:B:39:HIS:NE2	2.26	0.50
1:B:120:VAL:HG13	1:B:178:LEU:HD23	1.92	0.50
1:A:265:CYS:O	1:A:268:GLN:HB2	2.12	0.50
1:B:417:GLN:HB3	1:B:469:VAL:HG12	1.93	0.50
1:B:61:ASN:HB3	1:B:64:LYS:HD2	1.94	0.50
1:B:500:LYS:O	1:B:535:HIS:ND1	2.45	0.50
1:B:417:GLN:HB3	1:B:469:VAL:CG1	2.42	0.49
1:A:342:SER:CB	1:A:450:GLU:HG2	2.42	0.49
1:B:67:HIS:CE1	1:B:99:ASN:OD1	2.65	0.49
1:A:200:CYS:O	1:A:204:GLN:HG3	2.12	0.49
1:B:312:SER:O	1:B:315:VAL:HG23	2.13	0.49
1:B:333:GLU:O	1:B:336:ARG:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:517:SER:OG	1:B:520:GLU:HG3	2.12	0.49
1:A:16:GLU:O	1:A:20:LYS:HB2	2.12	0.49
1:B:160:ARG:HH22	1:B:188:GLU:CD	2.21	0.49
1:B:385:GLN:HG3	1:B:446:MET:HE2	1.95	0.49
1:B:475:LYS:O	1:B:479:GLU:HB2	2.12	0.48
1:A:305:LEU:HG	1:A:337:ARG:NH1	2.29	0.48
1:B:25:ILE:HD13	1:B:154:LEU:HD23	1.95	0.48
1:A:5:SER:HB3	1:A:8:ALA:HB3	1.95	0.48
1:A:459:GLN:O	1:A:463:LEU:HG	2.14	0.48
1:B:67:HIS:NE2	1:B:249:ASP:OD1	2.47	0.48
1:A:247:HIS:O	1:A:247:HIS:CG	2.67	0.48
1:B:378:LYS:HB2	1:B:379:PRO:HD3	1.95	0.47
1:A:268:GLN:OE1	1:A:276:LYS:HA	2.15	0.47
1:B:443:ALA:O	1:B:445:ARG:N	2.47	0.47
1:B:30:TYR:CE1	1:B:102:PHE:HB3	2.49	0.47
1:A:441:PRO:C	1:A:443:ALA:H	2.23	0.46
1:A:441:PRO:HD2	1:A:444:LYS:HD3	1.97	0.46
1:A:567:CYS:O	1:A:571:GLU:HB2	2.15	0.46
1:B:19:PHE:O	1:B:23:VAL:HG23	2.16	0.46
1:B:30:TYR:CD1	1:B:102:PHE:HB3	2.50	0.46
1:A:441:PRO:C	1:A:443:ALA:N	2.74	0.46
1:B:198:LEU:HA	1:B:458:ASN:ND2	2.31	0.46
1:A:485:ARG:NH2	1:A:486:PRO:HG3	2.29	0.46
1:B:317:LYS:O	1:B:321:GLU:HG3	2.16	0.46
1:B:536:LYS:O	1:B:536:LYS:HG2	2.14	0.46
1:A:554:PHE:HE1	1:A:571:GLU:HB2	1.81	0.46
1:B:165:PHE:O	1:B:169:CYS:SG	2.73	0.46
1:A:238:LEU:HD12	1:A:238:LEU:HA	1.63	0.46
1:A:238:LEU:O	1:A:241:VAL:HB	2.16	0.46
1:B:456:VAL:O	1:B:459:GLN:HB3	2.16	0.46
1:B:526:GLN:O	1:B:530:VAL:HG23	2.16	0.46
1:A:417:GLN:HB2	1:A:470:SER:HB3	1.96	0.46
1:A:38:ASP:O	1:A:42:LEU:HG	2.16	0.45
1:A:323:LYS:O	1:A:327:LEU:HG	2.16	0.45
1:B:231:VAL:O	1:B:235:VAL:HG23	2.15	0.45
1:B:408:LEU:HD23	1:B:529:LEU:HD23	1.97	0.45
1:A:23:VAL:HG12	1:A:43:VAL:HG22	1.99	0.45
1:B:279:CYS:HA	1:B:286:LYS:HD3	1.97	0.45
1:A:41:LYS:NZ	1:A:42:LEU:CD2	2.80	0.45
1:A:100:GLU:O	1:A:104:GLN:HB2	2.16	0.45
1:A:420:THR:N	1:A:421:PRO:CD	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:TYR:CE2	1:B:144:ARG:NH1	2.85	0.45
1:B:485:ARG:HB3	1:B:486:PRO:HD3	1.99	0.45
1:A:208:GLU:O	1:A:212:LYS:HG3	2.16	0.45
1:B:329:MET:O	1:B:333:GLU:HG2	2.17	0.45
1:B:275:LEU:HD23	1:B:293:VAL:HG21	1.99	0.44
1:A:186:ARG:NH1	1:A:190:LYS:HD3	2.32	0.44
1:B:137:LYS:HE2	1:B:137:LYS:HB2	1.83	0.44
1:A:408:LEU:HD23	1:A:427:SER:HB2	1.98	0.44
1:B:319:TYR:OH	1:B:358:GLU:HG2	2.17	0.44
1:A:312:SER:O	1:A:315:VAL:HG23	2.18	0.44
1:A:351:LYS:HA	1:A:351:LYS:HD2	1.81	0.44
1:A:437:CYS:HA	1:A:440:HIS:CD2	2.48	0.44
1:B:157:PHE:HE2	1:B:188:GLU:HB3	1.82	0.44
1:A:34:CYS:HA	1:A:35:PRO:HD3	1.88	0.44
1:A:353:TYR:HD1	1:A:373:VAL:HG11	1.82	0.44
1:A:41:LYS:NZ	1:A:42:LEU:HD23	2.33	0.44
1:A:572:GLY:O	1:A:576:VAL:HG13	2.17	0.44
1:A:533:VAL:C	1:A:535:HIS:H	2.26	0.44
1:B:81:ARG:HB2	1:B:85:GLY:HA2	2.00	0.43
1:A:467:THR:O	1:A:469:VAL:HG23	2.18	0.43
1:A:500:LYS:O	1:A:535:HIS:ND1	2.52	0.43
1:B:408:LEU:HD13	1:B:427:SER:HB2	1.99	0.43
1:B:567:CYS:O	1:B:571:GLU:HB2	2.19	0.43
1:A:49:PHE:O	1:A:50:ALA:C	2.61	0.43
1:A:349:LEU:HD23	1:A:380:LEU:HD12	2.00	0.43
1:B:378:LYS:O	1:B:379:PRO:C	2.59	0.43
1:A:41:LYS:O	1:A:45:GLU:HG3	2.17	0.43
1:A:353:TYR:O	1:A:356:THR:HB	2.17	0.43
1:A:509:PHE:HB2	1:A:568:PHE:HE1	1.83	0.43
1:B:160:ARG:NH2	1:B:188:GLU:OE2	2.52	0.43
1:A:543:GLN:O	1:A:547:VAL:HG23	2.18	0.43
1:B:452:TYR:O	1:B:456:VAL:HG23	2.18	0.43
1:A:137:LYS:O	1:A:141:GLU:HG2	2.19	0.43
1:A:196:GLN:HA	1:A:196:GLN:HE21	1.81	0.42
1:B:200:CYS:O	1:B:204:GLN:HG3	2.19	0.42
1:A:305:LEU:O	1:A:307:ALA:N	2.52	0.42
1:A:457:LEU:HD13	1:A:488:PHE:CD2	2.54	0.42
1:A:509:PHE:CB	1:A:568:PHE:HE1	2.31	0.42
1:B:327:LEU:HD23	1:B:327:LEU:HA	1.86	0.42
1:A:398:LEU:O	1:A:402:LYS:HD2	2.19	0.42
1:A:409:VAL:O	1:A:413:LYS:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:GLN:HG3	1:A:544:LEU:N	2.35	0.42
1:A:408:LEU:HD11	1:A:526:GLN:HB3	2.01	0.42
1:A:419:SER:OG	1:A:421:PRO:HD2	2.20	0.42
1:B:420:THR:N	1:B:421:PRO:CD	2.83	0.42
1:A:423:LEU:HD23	1:A:423:LEU:HA	1.87	0.42
1:B:84:TYR:O	1:B:85:GLY:C	2.63	0.42
1:B:378:LYS:HE3	1:B:378:LYS:HB3	1.84	0.42
1:A:506:THR:O	1:A:506:THR:HG22	2.20	0.42
1:A:536:LYS:HG2	1:A:536:LYS:O	2.18	0.42
1:B:543:GLN:HG3	1:B:544:LEU:N	2.35	0.42
1:A:554:PHE:HZ	1:A:568:PHE:O	2.03	0.41
1:A:118:PRO:HB2	1:A:122:VAL:HB	2.01	0.41
1:B:151:ALA:HB2	1:B:250:LEU:HD13	2.01	0.41
1:B:531:GLU:O	1:B:535:HIS:CD2	2.73	0.41
1:A:286:LYS:O	1:A:290:ILE:HG13	2.20	0.41
1:A:342:SER:HB2	1:A:450:GLU:HG2	2.03	0.41
1:B:218:ARG:HE	1:B:218:ARG:HA	1.85	0.41
1:A:72:ASP:O	1:A:76:THR:HG23	2.21	0.41
1:A:394:LEU:HD11	1:A:398:LEU:HD11	2.01	0.41
1:B:423:LEU:HD23	1:B:423:LEU:HA	1.93	0.41
1:A:45:GLU:OE1	1:A:73:LYS:HD2	2.20	0.41
1:A:30:TYR:HD1	1:A:30:TYR:HA	1.78	0.41
1:A:39:HIS:O	1:A:43:VAL:HG23	2.20	0.41
1:A:383:GLU:CD	1:A:485:ARG:HH22	2.28	0.41
1:A:60:GLU:HG2	1:A:61:ASN:ND2	2.35	0.41
1:A:464:HIS:CE1	1:A:469:VAL:H	2.38	0.41
1:B:168:CYS:SG	1:B:177:CYS:C	3.04	0.41
1:A:164:ALA:O	1:A:168:CYS:HB2	2.20	0.41
1:B:345:LEU:O	1:B:349:LEU:HG	2.20	0.41
1:B:6:GLU:O	1:B:9:HIS:HB3	2.20	0.41
1:B:513:ILE:HG12	1:B:521:ARG:HG3	2.03	0.41
1:B:551:PHE:HA	1:B:554:PHE:HB3	2.02	0.41
1:B:120:VAL:HG13	1:B:178:LEU:CD2	2.51	0.41
1:B:394:LEU:HD12	1:B:394:LEU:HA	1.88	0.41
1:B:543:GLN:O	1:B:546:ALA:HB3	2.21	0.41
1:A:383:GLU:OE1	1:A:485:ARG:NH2	2.51	0.40
1:A:98:ARG:O	1:A:101:CYS:HB3	2.21	0.40
1:B:441:PRO:C	1:B:443:ALA:N	2.76	0.40
1:B:564:LYS:O	1:B:565:GLU:HB2	2.21	0.40
1:A:61:ASN:OD1	1:A:64:LYS:NZ	2.40	0.40
1:A:348:ARG:O	1:A:352:THR:OG1	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:GLU:C	1:B:268:GLN:H	2.29	0.40
1:A:27:PHE:HZ	1:A:46:VAL:HG21	1.87	0.40
1:A:73:LYS:HD3	1:A:73:LYS:HA	1.88	0.40
1:A:249:ASP:HB3	1:A:252:GLU:HG2	2.03	0.40
1:B:81:ARG:C	1:B:83:THR:N	2.79	0.40
1:B:372:LYS:O	1:B:375:ASP:HB2	2.21	0.40
1:A:84:TYR:O	1:A:85:GLY:C	2.64	0.40
1:A:352:THR:O	1:A:353:TYR:C	2.63	0.40
1:B:123:MET:HB3	1:B:165:PHE:CE2	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	576/585 (98%)	519 (90%)	46 (8%)	11 (2%)	6	11
1	B	576/585 (98%)	530 (92%)	33 (6%)	13 (2%)	5	8
All	All	1152/1170 (98%)	1049 (91%)	79 (7%)	24 (2%)	5	9

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	GLU
1	A	501	GLU
1	B	60	GLU
1	B	442	GLU
1	B	444	LYS
1	B	501	GLU
1	A	59	ALA
1	A	85	GLY
1	A	306	ALA

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Mol	Chain	Res	Type
1	A	442	GLU
1	B	59	ALA
1	B	79	THR
1	B	85	GLY
1	B	321	GLU
1	B	373	VAL
1	B	566	THR
1	A	466	LYS
1	B	364	ALA
1	B	367	HIS
1	A	537	PRO
1	A	566	THR
1	A	171	ALA
1	A	175	ALA
1	B	416	PRO

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	506/511 (99%)	482 (95%)	24 (5%)	23	47
1	B	506/511 (99%)	479 (95%)	27 (5%)	20	42
All	All	1012/1022 (99%)	961 (95%)	51 (5%)	22	44

All (51) 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	79	THR
1	A	109	ASN
1	A	179	LEU
1	A	187	ASP
1	A	208	GLU

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Mol	Chain	Res	Type
1	A	252	GLU
1	A	271	ILE
1	A	276	LYS
1	A	294	GLU
1	A	375	ASP
1	A	392	CYS
1	A	414	LYS
1	A	435	SER
1	A	450	GLU
1	A	493	VAL
1	A	510	HIS
1	A	540	THR
1	A	548	MET
1	A	557	LYS
1	A	566	THR
1	A	567	CYS
1	B	34	CYS
1	B	58	SER
1	B	79	THR
1	B	89	ASP
1	B	121	ASP
1	B	137	LYS
1	B	144	ARG
1	B	187	ASP
1	B	208	GLU
1	B	218	ARG
1	B	219	LEU
1	B	245	CYS
1	B	276	LYS
1	B	293	VAL
1	B	308	ASP
1	B	310	VAL
1	B	324	ASP
1	B	375	ASP
1	B	435	SER
1	B	450	GLU
1	B	479	GLU
1	B	498	VAL
1	B	512	ASP
1	B	540	THR
1	B	544	LEU
1	B	548	MET

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Mol	Chain	Res	Type
1	B	557	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	109	ASN
1	A	170	GLN
1	A	196	GLN
1	A	386	ASN
1	A	440	HIS
1	A	464	HIS
1	A	580	GLN
1	B	33	GLN
1	B	196	GLN
1	B	385	GLN
1	B	386	ASN
1	B	390	GLN
1	B	440	HIS
1	B	483	ASN
1	B	580	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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%)	-0.08	24 (4%) 40 36	13, 36, 96, 106	0
1	B	578/585 (98%)	-0.10	22 (3%) 44 39	15, 38, 96, 109	0
All	All	1156/1170 (98%)	-0.09	46 (3%) 42 38	13, 37, 96, 109	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	582	ALA	4.8
1	B	501	GLU	4.2
1	B	86	GLU	3.9
1	A	575	LEU	3.8
1	B	505	GLU	3.8
1	A	560	LYS	3.7
1	B	78	ALA	3.7
1	B	84	TYR	3.6
1	A	84	TYR	3.6
1	B	582	ALA	3.6
1	B	565	GLU	3.3
1	A	87	MET	3.2
1	B	87	MET	3.2
1	A	499	PRO	3.0
1	B	539	ALA	2.9
1	B	506	THR	2.9
1	B	80	LEU	2.9
1	A	568	PHE	2.8
1	B	502	PHE	2.7
1	B	503	ASN	2.7
1	B	575	LEU	2.7
1	A	547	VAL	2.6
1	B	88	ALA	2.5
1	B	576	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	504	ALA	2.4
1	A	88	ALA	2.4
1	A	501	GLU	2.4
1	A	502	PHE	2.3
1	A	498	VAL	2.3
1	A	79	THR	2.3
1	A	443	ALA	2.3
1	A	538	LYS	2.2
1	A	503	ASN	2.2
1	B	511	ALA	2.2
1	A	540	THR	2.2
1	A	561	ALA	2.2
1	A	369	CYS	2.2
1	A	539	ALA	2.2
1	B	510	HIS	2.2
1	A	80	LEU	2.2
1	A	85	GLY	2.1
1	B	77	VAL	2.1
1	A	543	GLN	2.1
1	B	504	ALA	2.1
1	B	536	LYS	2.1
1	B	569	ALA	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.