



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 05:20 PM EDT

PDB ID : 8Y9T / pdb_00008y9t
Title : Crystal structure of nanobody MY6322 bound to human serum albumin (HSA)
Authors : Ding, Y.; Zhong, P.Y.
Deposited on : 2024-02-07
Resolution : 2.40 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

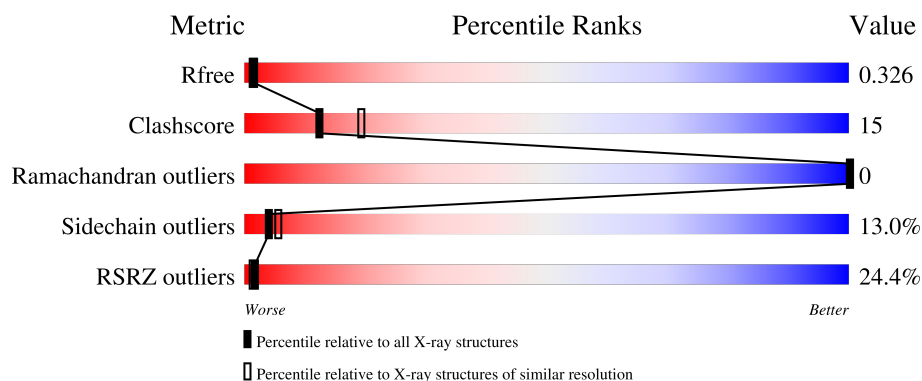
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	591	
2	B	126	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5356 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 Albumin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	543	Total	C	N	O	S	0	1	0
			4326	2735	726	826	39			

- Molecule 2 is a protein called nanobody MY6322.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	126	Total	C	N	O	S	0	2	0
			977	606	174	191	6			

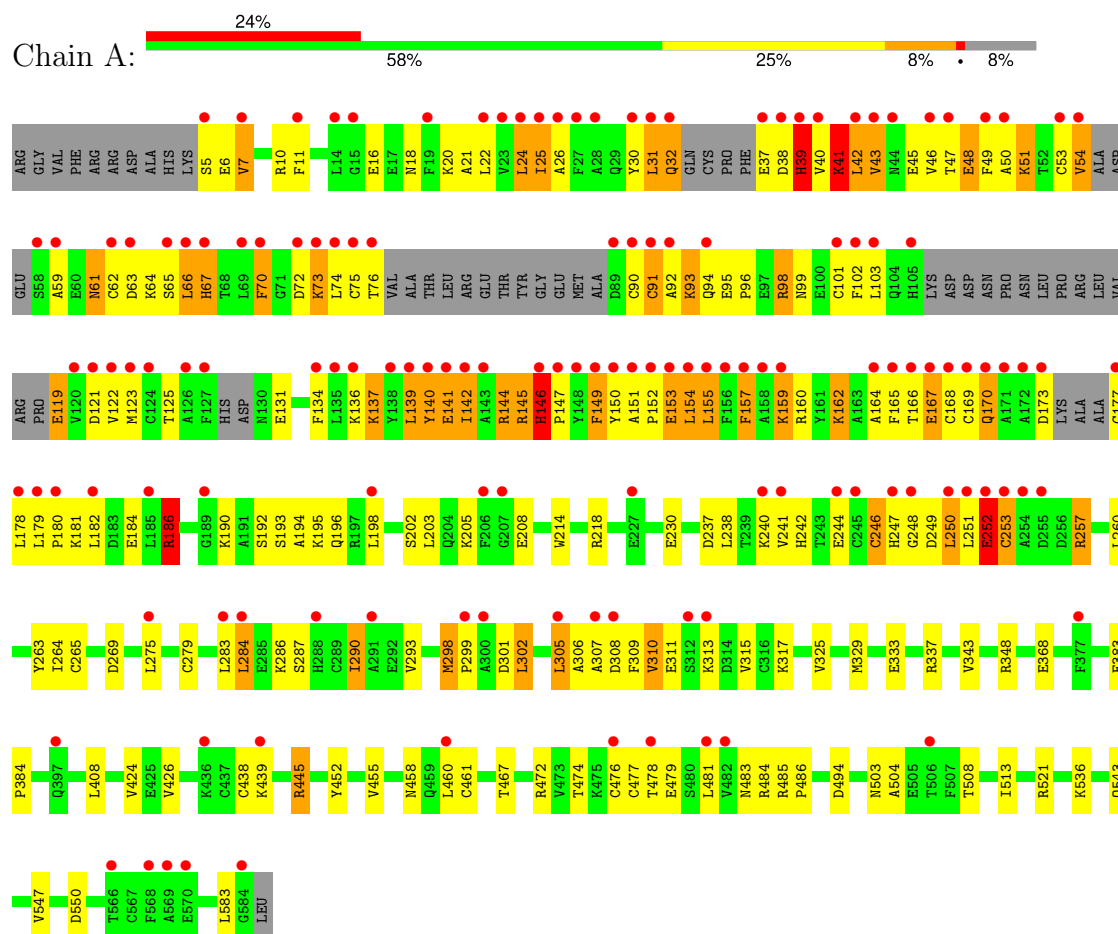
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	48	Total	O	0	0
			48	48		
3	B	5	Total	O	0	0
			5	5		

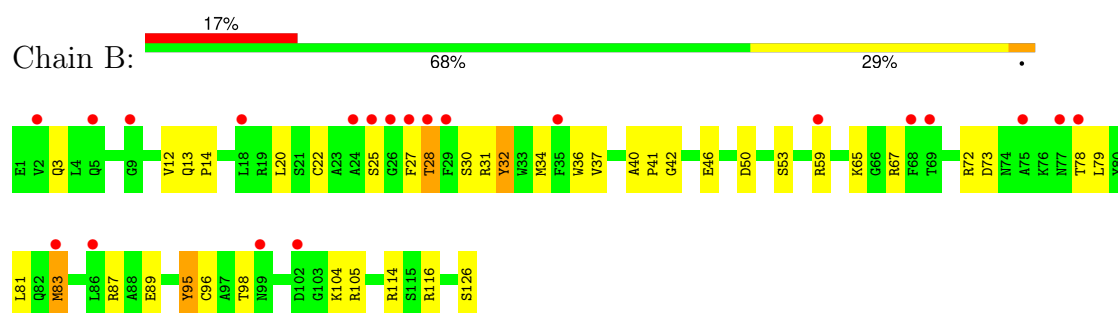
3 Residue-property plots

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: Albumin



• Molecule 2: nanobody MY6322



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	167.95Å 73.70Å 86.01Å 90.00° 118.74° 90.00°	Depositor
Resolution (Å)	75.41 – 2.40 75.41 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.1 (75.41-2.40) 99.1 (75.41-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.263 , 0.324 0.277 , 0.326	Depositor DCC
R_{free} test set	1807 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	55.2	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 66.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.019 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5356	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.60% 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](#)

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	0.72	0/4402	1.28	23/5924 (0.4%)
2	B	0.61	1/1003 (0.1%)	0.99	4/1351 (0.3%)
All	All	0.70	1/5405 (0.0%)	1.23	27/7275 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9
2	B	0	7
All	All	0	16

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	83	MET	SD-CE	-5.58	1.65	1.79

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	CYS	CB-CA-C	-14.25	87.14	110.79
2	B	32	TYR	N-CA-CB	-9.19	97.27	111.05
1	A	250	LEU	CA-C-N	-8.99	109.92	123.04
1	A	250	LEU	C-N-CA	-8.99	109.92	123.04
1	A	481	LEU	N-CA-CB	-8.09	98.23	110.12
1	A	315	VAL	N-CA-CB	-7.41	100.47	110.54
1	A	247	HIS	N-CA-C	-6.91	103.75	111.28
1	A	252	GLU	N-CA-CB	-6.86	100.04	110.12
1	A	39	HIS	CB-CA-C	6.48	121.50	110.56
1	A	246	CYS	N-CA-C	-6.37	104.34	111.28
1	A	147	PRO	N-CA-C	6.19	122.32	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	157	PHE	CA-CB-CG	6.03	119.83	113.80
1	A	476	CYS	CB-CA-C	5.86	120.51	110.79
2	B	32	TYR	N-CA-C	5.70	118.52	109.81
1	A	51	LYS	N-CA-C	-5.64	105.14	111.28
1	A	477	CYS	CA-C-N	5.61	127.79	120.28
1	A	477	CYS	C-N-CA	5.61	127.79	120.28
1	A	40	VAL	N-CA-C	-5.51	105.00	110.62
1	A	41	LYS	N-CA-C	-5.42	105.37	111.28
1	A	7	VAL	N-CA-C	-5.40	105.11	110.62
2	B	28	THR	N-CA-CB	-5.28	101.86	109.83
2	B	73	ASP	CA-CB-CG	5.26	117.86	112.60
1	A	146	HIS	CA-CB-CG	-5.22	108.58	113.80
1	A	242	HIS	CB-CA-C	5.14	119.60	110.85
1	A	247	HIS	CB-CA-C	5.13	119.30	110.79
1	A	170	GLN	CB-CA-C	5.08	119.22	110.79
1	A	309	PHE	CB-CA-C	5.05	115.68	109.16

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	144	ARG	Sidechain
1	A	145	ARG	Sidechain
1	A	160	ARG	Sidechain
1	A	186	ARG	Sidechain
1	A	218	ARG	Sidechain
1	A	348	ARG	Sidechain
1	A	445	ARG	Sidechain
1	A	472	ARG	Sidechain
1	A	521	ARG	Sidechain
2	B	105	ARG	Sidechain
2	B	116	ARG	Sidechain
2	B	31	ARG	Sidechain
2	B	59	ARG	Sidechain
2	B	67	ARG	Sidechain
2	B	72	ARG	Sidechain
2	B	87	ARG	Sidechain

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	4326	0	4270	139	0
2	B	977	0	937	18	0
3	A	48	0	0	3	0
3	B	5	0	0	1	0
All	All	5356	0	5207	157	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 15.

All (157) 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:461:CYS:SG	1:A:484:ARG:NH1	2.39	0.95
1:A:145:ARG:HD3	1:A:146:HIS:HB2	1.60	0.83
1:A:305:LEU:HD21	1:A:333:GLU:HB3	1.66	0.77
1:A:142:ILE:O	1:A:145:ARG:HG3	1.85	0.77
1:A:26:ALA:HB2	1:A:250:LEU:HD22	1.68	0.76
1:A:96:PRO:HA	1:A:99:ASN:HD22	1.52	0.73
1:A:306:ALA:HA	1:A:310:VAL:HG13	1.70	0.73
1:A:307:ALA:HA	1:A:311:GLU:HB2	1.71	0.72
1:A:149:PHE:HB3	1:A:154:LEU:HD11	1.70	0.72
1:A:287:SER:HA	1:A:290:ILE:HD13	1.73	0.71
1:A:95:GLU:HB3	1:A:96:PRO:HD2	1.73	0.69
2:B:30:SER:O	2:B:53:SER:HB2	1.92	0.69
1:A:290:ILE:O	1:A:293:VAL:HG12	1.93	0.69
1:A:192:SER:O	1:A:195:LYS:HG3	1.94	0.67
1:A:75:CYS:HG	1:A:91:CYS:HG	1.42	0.67
1:A:283:LEU:HD12	1:A:284:LEU:N	2.09	0.67
1:A:10:ARG:HH21	1:A:252:GLU:HB3	1.61	0.66
1:A:95:GLU:O	1:A:98:ARG:HG3	1.94	0.66
1:A:43:VAL:O	1:A:46:VAL:HG22	1.96	0.65
1:A:154:LEU:HA	1:A:157:PHE:CE2	2.33	0.63
1:A:20:LYS:HD2	1:A:47:THR:HG21	1.80	0.63
1:A:131:GLU:H	1:A:131:GLU:CD	2.07	0.62
2:B:42:GLY:N	3:B:201:HOH:O	2.20	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:ALA:O	1:A:308:ASP:HB2	1.99	0.62
1:A:164:ALA:O	1:A:167:GLU:HG3	2.00	0.61
1:A:137:LYS:HA	1:A:140:TYR:CD2	2.36	0.60
1:A:150:TYR:OH	1:A:241:VAL:HG12	2.01	0.60
1:A:137:LYS:HA	1:A:140:TYR:CE2	2.37	0.59
1:A:39:HIS:HB3	1:A:42:LEU:HD23	1.83	0.59
1:A:141:GLU:HG2	1:A:142:ILE:N	2.17	0.59
1:A:283:LEU:CD1	1:A:284:LEU:HD22	2.33	0.58
1:A:503:ASN:OD1	1:A:504:ALA:N	2.36	0.58
1:A:24:LEU:HG	1:A:139:LEU:HD21	1.84	0.57
1:A:48:GLU:HA	1:A:51:LYS:HD2	1.86	0.57
1:A:325:VAL:CG1	1:A:329:MET:HE3	2.35	0.57
1:A:50:ALA:O	1:A:53:CYS:SG	2.59	0.57
1:A:305:LEU:HD21	1:A:333:GLU:CB	2.35	0.56
1:A:164:ALA:HB2	1:A:181:LYS:HG2	1.87	0.56
1:A:93:LYS:O	1:A:95:GLU:HG3	2.06	0.56
1:A:265:CYS:SG	1:A:279:CYS:SG	3.01	0.55
1:A:159:LYS:O	1:A:162:LYS:HG3	2.07	0.55
1:A:186:ARG:HD2	1:A:190:LYS:HE2	1.88	0.55
1:A:275:LEU:O	1:A:279:CYS:SG	2.65	0.54
1:A:31:LEU:O	1:A:31:LEU:HG	2.08	0.54
1:A:42:LEU:O	1:A:45:GLU:HB3	2.09	0.53
1:A:265:CYS:SG	1:A:286:LYS:HD3	2.49	0.53
2:B:28:THR:O	2:B:28:THR:OG1	2.27	0.53
2:B:20:LEU:HG	2:B:83:MET:CE	2.39	0.52
1:A:59:ALA:HB3	1:A:62:CYS:SG	2.49	0.52
1:A:250:LEU:O	1:A:251:LEU:C	2.48	0.52
1:A:93:LYS:O	1:A:94:GLN:NE2	2.43	0.52
1:A:144:ARG:HG3	3:A:613:HOH:O	2.10	0.52
1:A:92:ALA:HB2	3:A:638:HOH:O	2.10	0.51
1:A:198:LEU:HD13	1:A:458:ASN:HB2	1.92	0.51
1:A:98:ARG:HD2	1:A:98:ARG:C	2.35	0.51
1:A:483:ASN:C	1:A:486:PRO:HD2	2.36	0.50
1:A:42:LEU:O	1:A:46:VAL:HG13	2.11	0.50
1:A:162:LYS:O	1:A:166:THR:HG23	2.11	0.50
1:A:164:ALA:O	1:A:168:CYS:SG	2.69	0.50
1:A:494:ASP:OD1	1:A:494:ASP:C	2.55	0.50
1:A:181:LYS:O	1:A:184:GLU:HB3	2.12	0.49
1:A:383:GLU:HB3	1:A:384:PRO:HD3	1.94	0.49
1:A:53:CYS:SG	1:A:54:VAL:HG22	2.52	0.49
1:A:73:LYS:HD3	1:A:74:LEU:HD12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:GLU:OE1	1:A:154:LEU:N	2.45	0.49
1:A:165:PHE:CE1	1:A:182:LEU:HD11	2.47	0.49
1:A:504:ALA:O	1:A:508:THR:HG23	2.12	0.49
1:A:67:HIS:CE1	1:A:99:ASN:HD21	2.31	0.49
1:A:30:TYR:CE1	1:A:102:PHE:HZ	2.30	0.49
1:A:179:LEU:HB2	1:A:180:PRO:HD3	1.94	0.48
2:B:34:MET:SD	2:B:98:THR:HB	2.53	0.48
2:B:27:PHE:CD2	2:B:32:TYR:HE2	2.31	0.48
1:A:474:THR:O	1:A:478:THR:HG23	2.12	0.48
2:B:3:GLN:HB2	2:B:25:SER:HB2	1.94	0.48
1:A:11:PHE:C	1:A:11:PHE:CD1	2.90	0.48
1:A:177:CYS:O	1:A:180:PRO:HD2	2.13	0.48
1:A:237:ASP:O	1:A:240:LYS:HG3	2.13	0.48
1:A:426:VAL:HG21	1:A:460:LEU:HD13	1.95	0.48
1:A:66:LEU:HD12	1:A:67:HIS:H	1.78	0.48
1:A:41:LYS:HA	1:A:41:LYS:HD3	1.58	0.47
1:A:62:CYS:O	1:A:63:ASP:HB3	2.14	0.47
1:A:49:PHE:HZ	1:A:61:ASN:O	1.98	0.47
1:A:66:LEU:H	1:A:66:LEU:HG	1.49	0.47
1:A:452:TYR:O	1:A:455:VAL:HG12	2.15	0.47
1:A:61:ASN:HA	1:A:64:LYS:HZ2	1.79	0.47
1:A:99:ASN:O	1:A:103:LEU:HG	2.14	0.47
1:A:260:LEU:C	1:A:260:LEU:HD23	2.40	0.46
1:A:123:MET:HB3	1:A:165:PHE:HE2	1.81	0.46
1:A:49:PHE:O	1:A:53:CYS:N	2.47	0.46
1:A:90:CYS:C	1:A:91:CYS:SG	2.99	0.46
1:A:16:GLU:O	1:A:20:LYS:HG3	2.15	0.46
1:A:67:HIS:HA	1:A:70:PHE:HD2	1.80	0.46
1:A:154:LEU:HD23	1:A:157:PHE:HZ	1.81	0.46
1:A:196:GLN:NE2	1:A:246:CYS:SG	2.89	0.46
2:B:36:TRP:CD1	2:B:81:LEU:HD13	2.51	0.46
1:A:244:GLU:HB3	1:A:249:ASP:OD1	2.16	0.46
1:A:146:HIS:NE2	3:A:601:HOH:O	2.35	0.45
2:B:22:CYS:O	2:B:78:THR:HA	2.15	0.45
1:A:21:ALA:O	1:A:25:ILE:HD12	2.16	0.45
1:A:214:TRP:CD1	1:A:343:VAL:HG11	2.51	0.45
1:A:142:ILE:H	1:A:142:ILE:HG12	1.53	0.45
1:A:177:CYS:C	1:A:180:PRO:HD2	2.41	0.45
1:A:154:LEU:HD23	1:A:157:PHE:CZ	2.51	0.45
1:A:134:PHE:HA	1:A:137:LYS:HD2	1.99	0.45
1:A:136:LYS:HA	1:A:139:LEU:HD23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:VAL:HG23	2:B:46:GLU:O	2.17	0.45
1:A:139:LEU:HG	1:A:140:TYR:N	2.30	0.45
1:A:186:ARG:HE	1:A:186:ARG:HB3	1.55	0.45
1:A:298:MET:HE2	1:A:298:MET:HB2	1.80	0.45
1:A:150:TYR:O	1:A:151:ALA:C	2.60	0.45
1:A:137:LYS:HE2	1:A:137:LYS:HB3	1.29	0.44
1:A:152:PRO:HB3	1:A:257:ARG:HD2	1.99	0.44
1:A:186:ARG:O	1:A:190:LYS:HD2	2.16	0.44
2:B:12:VAL:HG22	2:B:13:GLN:H	1.83	0.44
1:A:22:LEU:C	1:A:22:LEU:HD13	2.43	0.44
1:A:119:GLU:O	1:A:123:MET:HG3	2.18	0.44
1:A:302:LEU:HD12	1:A:302:LEU:HA	1.78	0.44
2:B:14:PRO:CD	2:B:126:SER:HA	2.48	0.44
1:A:194:ALA:HB1	1:A:455:VAL:HG23	2.00	0.43
1:A:195:LYS:O	1:A:198:LEU:HB3	2.18	0.43
1:A:20:LYS:CD	1:A:47:THR:HG21	2.48	0.43
1:A:438:CYS:O	1:A:445:ARG:NH2	2.47	0.43
1:A:305:LEU:HD11	1:A:333:GLU:HB2	2.00	0.43
1:A:20:LYS:O	1:A:24:LEU:HD22	2.19	0.43
1:A:299:PRO:HB2	1:A:302:LEU:HD13	1.99	0.43
1:A:155:LEU:HD13	1:A:155:LEU:N	2.34	0.43
1:A:10:ARG:HE	1:A:252:GLU:HA	1.84	0.43
1:A:61:ASN:HA	1:A:61:ASN:HD22	1.58	0.43
2:B:40:ALA:HB1	2:B:41:PRO:HD2	1.99	0.43
1:A:230:GLU:OE2	1:A:263:TYR:OH	2.30	0.42
2:B:104:LYS:O	2:B:114:ARG:HG2	2.19	0.42
1:A:134:PHE:O	1:A:137:LYS:HG2	2.19	0.42
1:A:253:CYS:O	1:A:257:ARG:N	2.44	0.42
1:A:543:GLN:HB3	1:A:583:LEU:HD21	2.00	0.42
1:A:152:PRO:HA	1:A:155:LEU:HD22	2.00	0.42
1:A:260:LEU:HD23	1:A:264:ILE:HD13	2.00	0.42
2:B:65:LYS:HD2	2:B:65:LYS:C	2.44	0.42
1:A:73:LYS:O	1:A:74:LEU:C	2.63	0.42
1:A:151:ALA:O	1:A:154:LEU:HB2	2.20	0.42
2:B:36:TRP:HE3	2:B:95:TYR:O	2.03	0.41
1:A:30:TYR:CD1	1:A:102:PHE:HZ	2.38	0.41
1:A:287:SER:HA	1:A:290:ILE:CD1	2.47	0.41
1:A:149:PHE:HB3	1:A:154:LEU:CD1	2.44	0.41
2:B:89:GLU:N	2:B:89:GLU:OE1	2.51	0.41
1:A:536:LYS:NZ	1:A:583:LEU:O	2.36	0.41
1:A:408:LEU:HD21	1:A:424:VAL:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:LEU:HD11	1:A:284:LEU:HD22	2.03	0.41
1:A:317:LYS:HE3	1:A:317:LYS:HB3	1.84	0.41
2:B:34:MET:HB3	2:B:79:LEU:HD22	2.02	0.41
1:A:547:VAL:O	1:A:550:ASP:HB2	2.20	0.41
1:A:61:ASN:HA	1:A:64:LYS:HG3	2.02	0.40
1:A:244:GLU:O	1:A:248:GLY:N	2.55	0.40
1:A:250:LEU:O	1:A:251:LEU:HB2	2.22	0.40
1:A:337:ARG:HG3	1:A:337:ARG:HH11	1.85	0.40
1:A:485:ARG:HB3	1:A:486:PRO:HD3	2.03	0.40
1:A:31:LEU:C	1:A:32:GLN:HG2	2.46	0.40
1:A:140:TYR:CD1	1:A:141:GLU:N	2.89	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	529/591 (90%)	504 (95%)	25 (5%)	0	100	100
2	B	126/126 (100%)	122 (97%)	4 (3%)	0	100	100
All	All	655/717 (91%)	626 (96%)	29 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	477/516 (92%)	405 (85%)	72 (15%)	3	3
2	B	103/101 (102%)	100 (97%)	3 (3%)	37	60
All	All	580/617 (94%)	505 (87%)	75 (13%)	4	6

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	6	GLU
1	A	7	VAL
1	A	18	ASN
1	A	24	LEU
1	A	25	ILE
1	A	31	LEU
1	A	32	GLN
1	A	37	GLU
1	A	38	ASP
1	A	39	HIS
1	A	41	LYS
1	A	42	LEU
1	A	43	VAL
1	A	48	GLU
1	A	54	VAL
1	A	61	ASN
1	A	65	SER
1	A	66	LEU
1	A	67	HIS
1	A	70	PHE
1	A	72	ASP
1	A	73	LYS
1	A	76	THR
1	A	91	CYS
1	A	93	LYS
1	A	98	ARG
1	A	101	CYS
1	A	119	GLU
1	A	121	ASP
1	A	122	VAL
1	A	125	THR
1	A	137	LYS
1	A	139	LEU
1	A	140	TYR

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Mol	Chain	Res	Type
1	A	141	GLU
1	A	142	ILE
1	A	146	HIS
1	A	149	PHE
1	A	153	GLU
1	A	154	LEU
1	A	155	LEU
1	A	159	LYS
1	A	162	LYS
1	A	167	GLU
1	A	169	CYS
1	A	170	GLN
1	A	173	ASP
1	A	178	LEU
1	A	186	ARG
1	A	193	SER
1	A	202	SER
1	A	203	LEU
1	A	205	LYS
1	A	208	GLU
1	A	238	LEU
1	A	252	GLU
1	A	257	ARG
1	A	269	ASP
1	A	284	LEU
1	A	290	ILE
1	A	298	MET
1	A	301	ASP
1	A	302	LEU
1	A	305	LEU
1	A	310	VAL
1	A	313	LYS
1	A	368	GLU
1	A	439	LYS
1	A	467	THR
1	A	479	GLU
1	A	513	ILE
2	B	50	ASP
2	B	95	TYR
2	B	96	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	29	GLN
1	A	32	GLN
1	A	44	ASN
1	A	61	ASN
1	A	94	GLN
1	A	99	ASN
1	A	130	ASN
1	A	170	GLN
1	A	242	HIS
1	A	386	ASN
1	A	440	HIS
1	A	510	HIS
2	B	74	ASN
2	B	84	ASN

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	543/591 (91%)	1.33	142 (26%)  	40, 75, 155, 188	1 (0%)
2	B	126/126 (100%)	1.17	21 (16%)  	39, 66, 83, 105	2 (1%)
All	All	669/717 (93%)	1.30	163 (24%)  	39, 70, 152, 188	3 (0%)

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	139	LEU	8.2
1	A	70	PHE	8.1
1	A	135	LEU	6.4
1	A	251	LEU	6.2
1	A	40	VAL	6.0
1	A	156	PHE	6.0
1	A	31	LEU	6.0
1	A	120	VAL	5.8
1	A	72	ASP	5.4
1	A	43	VAL	5.3
1	A	179	LEU	5.2
1	A	150	TYR	5.1
1	A	69	LEU	5.0
1	A	66	LEU	5.0
1	A	103	LEU	4.8
1	A	7	VAL	4.5
1	A	54	VAL	4.3
1	A	143	ALA	4.3
1	A	22	LEU	4.3
1	A	94	GLN	4.2
1	A	253	CYS	4.2
1	A	157	PHE	4.2
1	A	178	LEU	4.2
1	A	122	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	149	PHE	4.0
1	A	164	ALA	4.0
1	A	47	THR	4.0
1	A	250	LEU	3.9
2	B	29	PHE	3.8
1	A	46	VAL	3.7
1	A	74	LEU	3.6
1	A	158	ALA	3.6
2	B	27	PHE	3.6
1	A	248	GLY	3.5
1	A	148	TYR	3.5
1	A	105	HIS	3.5
1	A	14	LEU	3.5
1	A	247	HIS	3.5
1	A	24	LEU	3.4
1	A	53	CYS	3.4
1	A	142	ILE	3.4
1	A	155	LEU	3.4
1	A	313	LYS	3.3
1	A	32	GLN	3.3
1	A	26	ALA	3.3
1	A	206	PHE	3.3
1	A	173	ASP	3.3
1	A	127	PHE	3.2
1	A	91	CYS	3.2
1	A	25	ILE	3.2
1	A	170	GLN	3.2
1	A	307	ALA	3.2
1	A	11	PHE	3.2
1	A	102	PHE	3.2
1	A	252	GLU	3.2
1	A	37	GLU	3.1
1	A	23	VAL	3.1
1	A	152	PRO	3.1
1	A	126	ALA	3.1
1	A	92	ALA	3.0
1	A	27	PHE	3.0
1	A	172	ALA	3.0
1	A	275	LEU	3.0
1	A	169	CYS	3.0
1	A	5	SER	3.0
1	A	76	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	568	PHE	3.0
2	B	83	MET	2.9
1	A	284	LEU	2.9
1	A	153	GLU	2.9
1	A	283	LEU	2.9
1	A	481	LEU	2.9
2	B	18	LEU	2.9
1	A	89	ASP	2.9
1	A	123	MET	2.9
1	A	439	LYS	2.8
1	A	569	ALA	2.8
1	A	185	LEU	2.8
2	B	35	PHE	2.8
1	A	42	LEU	2.8
1	A	245	CYS	2.8
1	A	154	LEU	2.8
1	A	171	ALA	2.8
2	B	77	ASN	2.7
1	A	19	PHE	2.7
1	A	138	TYR	2.7
1	A	167	GLU	2.7
1	A	288	HIS	2.7
1	A	15	GLY	2.7
1	A	397	GLN	2.7
1	A	62	CYS	2.6
1	A	134	PHE	2.6
2	B	68	PHE	2.6
1	A	241	VAL	2.6
1	A	50	ALA	2.6
2	B	24	ALA	2.6
1	A	39	HIS	2.6
1	A	90	CYS	2.6
1	A	151	ALA	2.6
2	B	75	ALA	2.5
1	A	121	ASP	2.5
1	A	299	PRO	2.5
1	A	49	PHE	2.5
2	B	28	THR	2.5
1	A	101	CYS	2.4
1	A	124	CYS	2.4
1	A	180	PRO	2.4
1	A	476	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	5	GLN	2.4
1	A	377	PHE	2.4
1	A	28	ALA	2.4
1	A	136	LYS	2.4
1	A	460	LEU	2.4
2	B	99	ASN	2.4
1	A	254	ALA	2.4
1	A	141	GLU	2.4
1	A	166	THR	2.3
1	A	227	GLU	2.3
1	A	147	PRO	2.3
1	A	58[A]	SER	2.3
2	B	2	VAL	2.3
1	A	312	SER	2.3
1	A	566	THR	2.3
1	A	59	ALA	2.2
1	A	67	HIS	2.2
1	A	73	LYS	2.2
1	A	305	LEU	2.2
1	A	165	PHE	2.2
1	A	300	ALA	2.2
1	A	75	CYS	2.2
1	A	38	ASP	2.2
1	A	198	LEU	2.2
1	A	584	GLY	2.2
1	A	436	LYS	2.2
1	A	168	CYS	2.2
1	A	189	GLY	2.2
1	A	570	GLU	2.2
1	A	482	VAL	2.1
1	A	506	THR	2.1
2	B	78	THR	2.1
2	B	86	LEU	2.1
1	A	63	ASP	2.1
1	A	44	ASN	2.1
2	B	9	GLY	2.1
1	A	291	ALA	2.1
1	A	182	LEU	2.1
1	A	177	CYS	2.1
1	A	308	ASP	2.1
1	A	207	GLY	2.1
2	B	26	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	244	GLU	2.1
1	A	140	TYR	2.1
2	B	102	ASP	2.1
1	A	65	SER	2.1
2	B	59	ARG	2.0
1	A	478	THR	2.0
2	B	25	SER	2.0
1	A	159	LYS	2.0
1	A	240	LYS	2.0
2	B	69	THR	2.0
1	A	255	ASP	2.0
1	A	30	TYR	2.0
1	A	146	HIS	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.