Full wwPDB X-ray Structure Validation Report ⓘ

Feb 3, 2025 – 12:27 PM JST

PDB ID	:	8Y9S
Title	:	Crystal structure of nanobody MY6321 bound to human serum albumin (HSA)
Authors	:	Ding, Y.; Zhong, P.Y.
Deposited on	:	2024-02-07
Resolution	:	2.88 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:

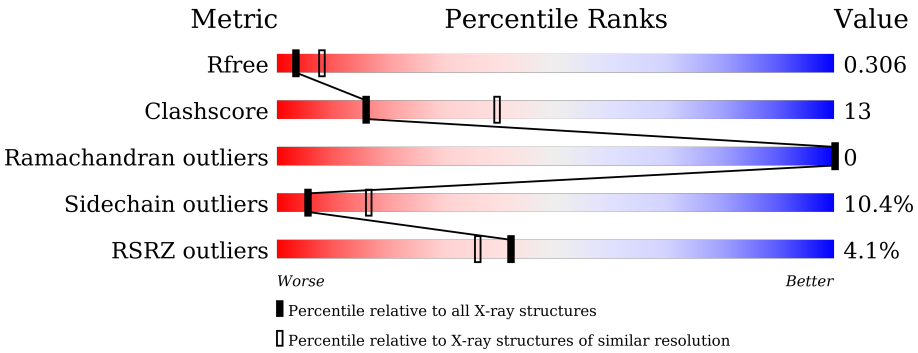
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.88 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}	164625	3316 (2.90-2.86)
Clashscore	180529	3609 (2.90-2.86)
Ramachandran outliers	177936	3529 (2.90-2.86)
Sidechain outliers	177891	3532 (2.90-2.86)
RSRZ outliers	164620	3319 (2.90-2.86)

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 <=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	4% 63% 27% 5%
1	C	591	5% 64% 26% 6%
2	B	122	% 66% 29%
2	D	122	2% 74% 25%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10913 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	567	Total	C	N	O	S	0	1	0
			4523	2857	764	861	41			
1	C	571	Total	C	N	O	S	0	1	0
			4546	2873	766	867	40			

- Molecule 2 is a protein called nanobody MY6321.

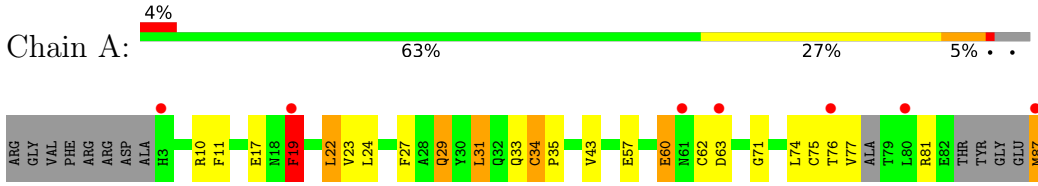
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	122	Total	C	N	O	S	0	0	0
			922	580	156	180	6			
2	D	122	Total	C	N	O	S	0	0	0
			922	580	156	180	6			

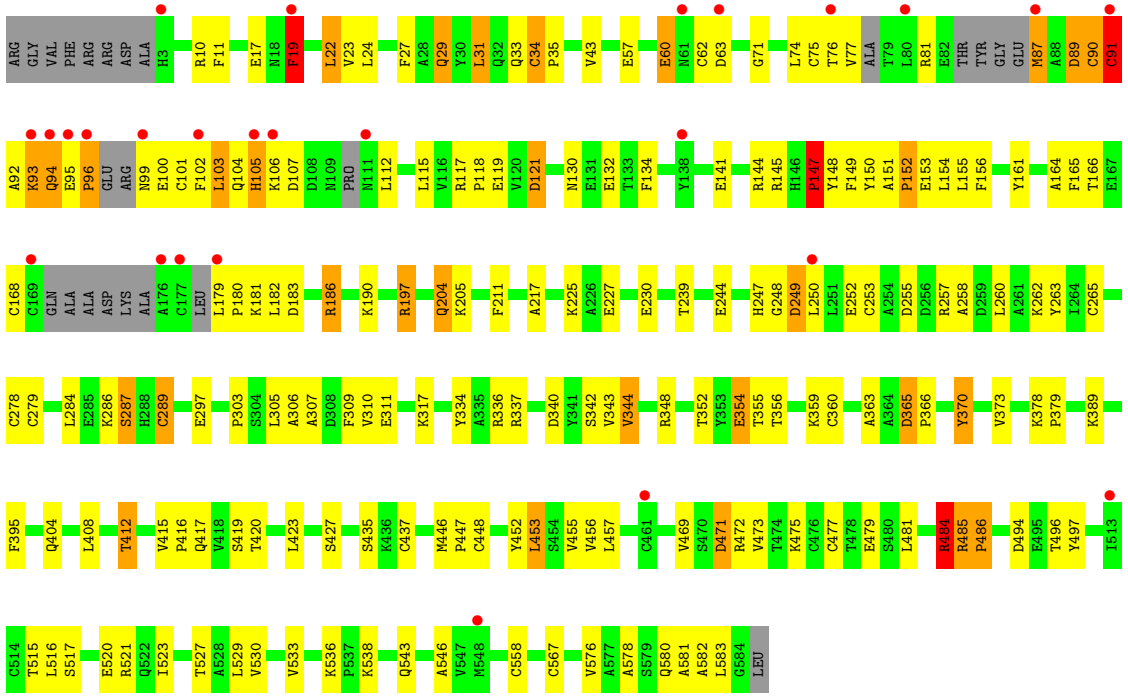
3 Residue-property plots (i)

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

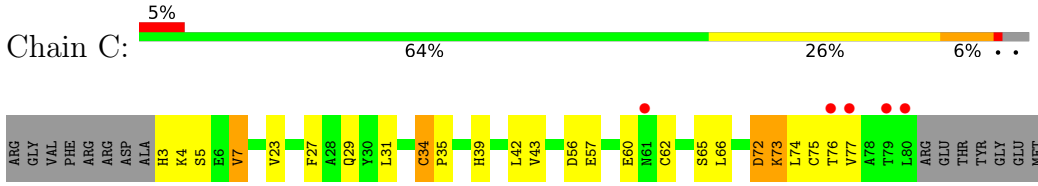
Chain A:

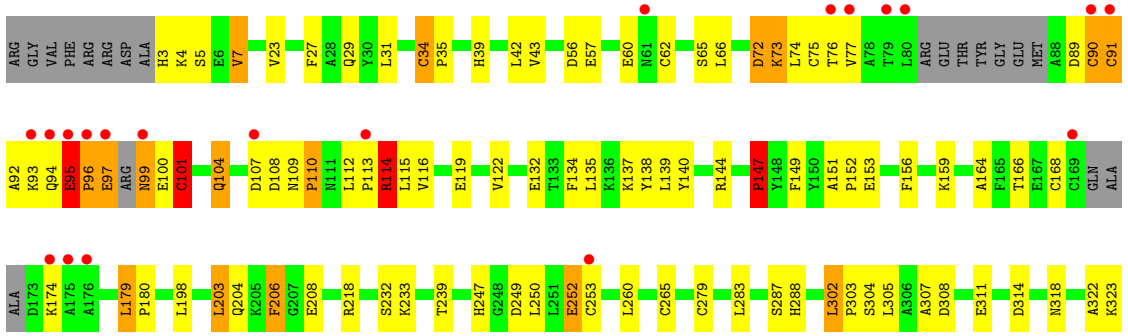


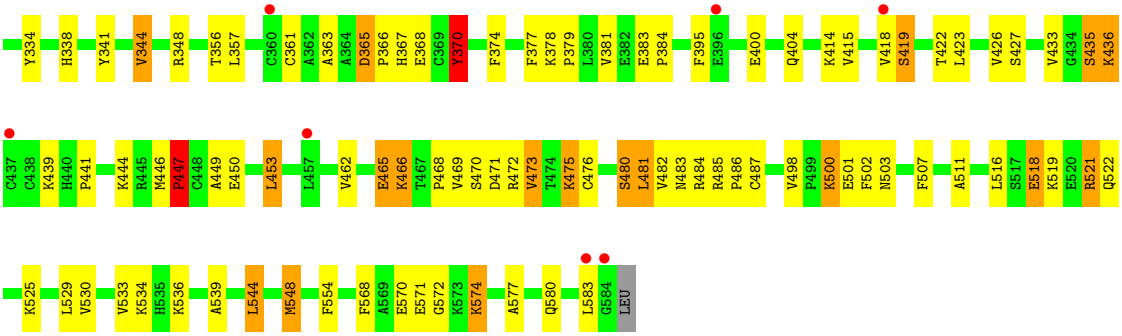


• Molecule 1: Albumin

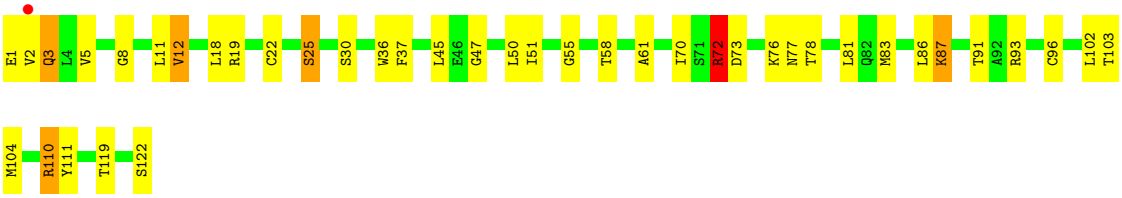
Chain C:



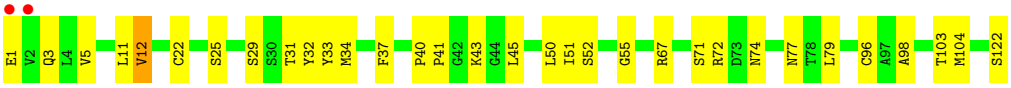




• Molecule 2: nanobody MY6321



• Molecule 2: nanobody MY6321



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	65.26Å 143.90Å 93.67Å 90.00° 100.23° 90.00°	Depositor
Resolution (Å)	46.25 – 2.88 46.25 – 2.88	Depositor EDS
% Data completeness (in resolution range)	99.3 (46.25-2.88) 99.3 (46.25-2.88)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.230 , 0.293 0.253 , 0.306	Depositor DCC
R_{free} test set	1820 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å^2)	63.3	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 50.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	10913	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 10.05% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.49	0/4605	0.97	21/6200 (0.3%)
1	C	0.50	0/4632	0.97	17/6244 (0.3%)
2	B	0.51	0/942	0.91	1/1277 (0.1%)
2	D	0.41	0/942	0.83	0/1277
All	All	0.49	0/11121	0.96	39/14998 (0.3%)

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	12
1	C	0	6
2	B	0	3
2	D	0	1
All	All	0	22

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	548	MET	CG-SD-CE	9.57	115.52	100.20
1	A	253	CYS	CB-CA-C	-8.90	92.61	110.40
1	A	484	ARG	CB-CA-C	-8.52	93.37	110.40
1	A	309	PHE	N-CA-CB	-8.36	95.56	110.60
1	C	62	CYS	CB-CA-C	8.18	126.76	110.40
1	A	370	TYR	N-CA-CB	7.98	124.97	110.60
1	A	370	TYR	CA-CB-CG	7.67	127.97	113.40
1	C	253	CYS	CB-CA-C	-7.57	95.25	110.40
1	C	370	TYR	CA-CB-CG	7.48	127.62	113.40
1	A	62	CYS	CB-CA-C	7.35	125.10	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	168	CYS	CB-CA-C	7.20	124.79	110.40
1	C	447	PRO	N-CA-CB	-7.05	94.84	103.30
1	A	150	TYR	N-CA-CB	-6.86	98.25	110.60
1	C	95	GLU	N-CA-CB	-6.76	98.44	110.60
1	C	90	CYS	CB-CA-C	-6.67	97.06	110.40
1	A	90	CYS	CB-CA-C	-6.67	97.07	110.40
1	C	468	PRO	N-CA-CB	-6.46	95.50	102.60
1	C	96	PRO	N-CA-C	-6.29	95.74	112.10
1	A	134	PHE	N-CA-CB	-6.28	99.30	110.60
1	A	19	PHE	N-CA-CB	-6.24	99.37	110.60
1	A	60	GLU	CB-CA-C	-6.20	98.01	110.40
1	C	370	TYR	N-CA-CB	5.98	121.37	110.60
1	C	110	PRO	N-CA-C	-5.90	96.75	112.10
1	A	147	PRO	N-CA-CB	-5.83	96.19	102.60
1	A	91	CYS	CA-CB-SG	-5.75	103.64	114.00
1	C	101	CYS	CB-CA-C	-5.71	98.97	110.40
1	C	247	HIS	CB-CA-C	5.71	121.81	110.40
1	A	152	PRO	N-CA-CB	-5.59	96.45	102.60
1	C	147	PRO	N-CA-CB	-5.54	96.50	102.60
1	A	484	ARG	N-CA-CB	-5.50	100.69	110.60
1	C	134	PHE	N-CA-CB	-5.47	100.75	110.60
1	A	252	GLU	N-CA-CB	-5.34	100.99	110.60
1	A	29	GLN	CB-CA-C	5.31	121.01	110.40
1	C	206	PHE	N-CA-CB	-5.29	101.08	110.60
1	C	507	PHE	CB-CA-C	5.21	120.81	110.40
1	A	96	PRO	N-CA-CB	-5.14	96.94	102.60
1	A	247	HIS	CB-CA-C	5.13	120.66	110.40
2	B	3	GLN	CB-CA-C	-5.08	100.24	110.40
1	A	180	PRO	N-CA-C	-5.07	98.92	112.10

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	144	ARG	Sidechain
1	A	186	ARG	Sidechain
1	A	197	ARG	Sidechain
1	A	336	ARG	Sidechain
1	A	337	ARG	Sidechain
1	A	472	ARG	Sidechain
1	A	484	ARG	Sidechain
1	A	485	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	57	GLU	Mainchain
1	A	582	ALA	Peptide
1	A	81	ARG	Sidechain
2	B	110	ARG	Sidechain
2	B	19	ARG	Sidechain
2	B	72	ARG	Sidechain
1	C	114	ARG	Sidechain
1	C	218	ARG	Sidechain
1	C	484	ARG	Sidechain
1	C	521	ARG	Sidechain
1	C	57	GLU	Mainchain
2	D	67	ARG	Sidechain

5.2 Too-close contacts (i)

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	4523	0	4453	120	1
1	C	4546	0	4479	109	2
2	B	922	0	901	29	1
2	D	922	0	901	21	0
All	All	10913	0	10734	275	2

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 13.

All (275) 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:408:LEU:O	1:A:412:THR:HG23	1.55	1.04
1:C:418:VAL:HG13	1:C:423:LEU:HD11	1.48	0.96
1:A:412:THR:HG22	1:A:423:LEU:HD23	1.53	0.90
1:A:265:CYS:HG	1:A:279:CYS:HG	1.19	0.89
1:A:95:GLU:HB2	1:A:99:ASN:N	1.90	0.87
1:C:415:VAL:O	1:C:418:VAL:HG12	1.77	0.85
1:C:90:CYS:HB3	1:C:101:CYS:HG	1.43	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:22:CYS:HG	2:B:96:CYS:HG	0.90	0.83
1:A:437:CYS:HG	1:A:448:CYS:HG	1.22	0.82
1:A:71:GLY:HA3	1:A:94:GLN:HB3	1.62	0.81
2:D:32:TYR:HD2	2:D:98:ALA:HB1	1.50	0.77
1:A:11:PHE:HD1	1:A:19:PHE:CD2	2.03	0.77
2:B:50:LEU:HD11	2:B:104:MET:HG2	1.67	0.76
1:A:558:CYS:HG	1:A:567:CYS:HG	1.26	0.76
1:A:536:LYS:HE3	1:A:583:LEU:HD13	1.68	0.76
1:C:90:CYS:HB3	1:C:101:CYS:SG	2.27	0.74
1:A:75:CYS:SG	1:A:91:CYS:O	2.46	0.74
2:D:22:CYS:HG	2:D:96:CYS:HG	0.75	0.73
1:C:110:PRO:HB2	1:C:112:LEU:HG	1.73	0.71
1:A:11:PHE:HD1	1:A:19:PHE:CE2	2.10	0.70
2:D:50:LEU:HD11	2:D:104:MET:HG2	1.73	0.70
1:A:342:SER:HB3	1:A:446:MET:HG2	1.73	0.69
1:C:90:CYS:CB	1:C:101:CYS:HG	2.06	0.68
1:A:265:CYS:HG	1:A:279:CYS:CB	2.07	0.68
1:A:101:CYS:O	1:A:105:HIS:HB2	1.93	0.68
1:A:412:THR:HG22	1:A:423:LEU:CD2	2.22	0.67
1:C:470:SER:HB3	1:C:473:VAL:HG12	1.76	0.67
2:D:5:VAL:O	2:D:22:CYS:HA	1.95	0.66
1:C:303:PRO:HG3	2:D:33:TYR:HE2	1.59	0.66
2:B:11:LEU:HD23	2:B:12:VAL:N	2.10	0.66
1:A:303:PRO:HG3	2:B:102:LEU:HD22	1.78	0.66
2:B:91:THR:HG23	2:B:119:THR:HA	1.77	0.66
1:C:395:PHE:CZ	1:C:435:SER:HA	2.32	0.65
1:A:204:GLN:HG2	1:A:205:LYS:N	2.11	0.65
1:C:383:GLU:HB3	1:C:384:PRO:HD3	1.78	0.64
1:C:449:ALA:O	1:C:453:LEU:HB2	1.98	0.64
1:A:100:GLU:HA	1:A:103:LEU:HD12	1.80	0.64
1:A:419:SER:O	1:A:423:LEU:HD12	1.98	0.64
2:B:37:PHE:HB3	2:B:45:LEU:HD12	1.81	0.63
1:A:516:LEU:O	1:A:521:ARG:NH2	2.33	0.62
2:B:51:ILE:HD11	2:B:55:GLY:HA2	1.81	0.62
2:B:73:ASP:HB3	2:B:76:LYS:HB2	1.81	0.62
2:D:50:LEU:HD11	2:D:104:MET:CG	2.30	0.61
1:A:161:TYR:CE1	1:A:165:PHE:HE2	2.19	0.61
1:C:164:ALA:O	1:C:168:CYS:HB2	2.01	0.61
1:A:408:LEU:HD12	1:A:427:SER:HB3	1.82	0.60
2:B:5:VAL:O	2:B:22:CYS:HA	2.01	0.60
1:C:72:ASP:O	1:C:76:THR:HG23	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:307:ALA:HA	1:C:311:GLU:HB2	1.85	0.59
1:A:11:PHE:CD1	1:A:19:PHE:CD2	2.87	0.59
1:A:225:LYS:HE3	1:A:297:GLU:O	2.01	0.59
1:C:75:CYS:SG	1:C:91:CYS:O	2.60	0.59
1:C:481:LEU:HG	1:C:482:VAL:N	2.18	0.59
1:C:418:VAL:HA	1:C:469:VAL:HG11	1.85	0.58
1:C:577:ALA:O	1:C:580:GLN:HG2	2.04	0.58
1:C:203:LEU:HD23	1:C:204:GLN:HG3	1.87	0.57
1:A:89:ASP:OD1	1:A:89:ASP:N	2.36	0.57
1:A:257:ARG:CZ	1:A:287:SER:HB2	2.35	0.57
1:A:258:ALA:O	1:A:262:LYS:HG3	2.04	0.57
1:C:153:GLU:OE2	1:C:288:HIS:ND1	2.38	0.57
1:A:19:PHE:CD1	1:A:19:PHE:C	2.79	0.56
1:A:99:ASN:O	1:A:102:PHE:N	2.38	0.56
1:A:103:LEU:O	1:A:104:GLN:HG2	2.05	0.56
1:C:414:LYS:O	1:C:472:ARG:NH2	2.38	0.56
1:A:27:PHE:CD1	1:A:74:LEU:HD21	2.41	0.56
2:D:34:MET:CE	2:D:72:ARG:NH2	2.69	0.56
1:A:257:ARG:NH1	1:A:287:SER:HB2	2.21	0.55
1:A:378:LYS:HB3	1:A:379:PRO:HD3	1.87	0.55
1:A:517:SER:OG	1:A:520:GLU:HG2	2.07	0.55
1:C:90:CYS:CB	1:C:101:CYS:SG	2.93	0.55
1:C:249:ASP:HB3	1:C:252:GLU:HG3	1.87	0.55
2:B:3:GLN:HE21	2:B:25:SER:HB2	1.72	0.55
1:C:539:ALA:HB3	1:C:544:LEU:HD11	1.88	0.55
1:A:307:ALA:HA	1:A:311:GLU:HB2	1.90	0.54
1:C:314:ASP:HB3	1:C:318:ASN:OD1	2.07	0.54
1:C:415:VAL:HG23	1:C:418:VAL:CG1	2.37	0.54
2:D:37:PHE:HB3	2:D:45:LEU:HD12	1.89	0.54
1:C:363:ALA:O	1:C:366:PRO:HG3	2.08	0.54
1:A:117:ARG:NH2	1:A:183:ASP:OD1	2.41	0.54
1:A:91:CYS:O	1:A:92:ALA:C	2.45	0.53
2:D:79:LEU:HD23	2:D:96:CYS:SG	2.49	0.53
1:A:404:GLN:O	1:A:408:LEU:HD12	2.08	0.53
2:B:1:GLU:HG2	2:B:3:GLN:OE1	2.09	0.53
1:C:322:ALA:O	1:C:323:LYS:C	2.47	0.53
2:B:50:LEU:HD11	2:B:104:MET:CG	2.37	0.53
1:C:511:ALA:HA	1:C:568:PHE:CE2	2.44	0.53
1:A:365:ASP:N	1:A:366:PRO:HD3	2.24	0.53
1:C:179:LEU:N	1:C:180:PRO:HD2	2.24	0.53
1:C:415:VAL:O	1:C:415:VAL:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:PHE:C	1:A:19:PHE:HD1	2.13	0.52
1:C:554:PHE:HE1	1:C:571:GLU:C	2.12	0.52
1:A:485:ARG:HB3	1:A:486:PRO:HD3	1.91	0.52
1:A:278:CYS:HB3	1:A:289:CYS:HB3	1.90	0.52
1:C:400:GLU:O	1:C:404:GLN:HG3	2.09	0.52
1:C:100:GLU:O	1:C:104:GLN:N	2.41	0.52
1:C:365:ASP:N	1:C:366:PRO:HD3	2.25	0.52
1:A:217:ALA:HB3	1:A:343:VAL:HG13	1.91	0.51
1:A:23:VAL:HG12	1:A:43:VAL:HG22	1.93	0.51
1:C:90:CYS:SG	1:C:91:CYS:N	2.84	0.51
1:C:303:PRO:HG3	2:D:33:TYR:CE2	2.44	0.51
2:B:102:LEU:O	2:B:102:LEU:HG	2.10	0.51
1:C:27:PHE:CD1	1:C:74:LEU:HD21	2.45	0.50
1:C:378:LYS:HB3	1:C:379:PRO:HD3	1.92	0.50
2:B:8:GLY:O	2:B:18:LEU:HD22	2.11	0.50
2:B:2:VAL:HA	2:B:25:SER:O	2.11	0.50
1:C:265:CYS:HG	1:C:279:CYS:CB	2.21	0.50
1:A:100:GLU:O	1:A:104:GLN:NE2	2.45	0.50
1:A:363:ALA:O	1:A:366:PRO:HG3	2.12	0.49
1:C:95:GLU:HB2	1:C:97:GLU:C	2.31	0.49
1:A:408:LEU:CD1	1:A:427:SER:HB3	2.43	0.49
1:C:422:THR:O	1:C:426:VAL:HG23	2.12	0.49
2:B:83:MET:HB3	2:B:86:LEU:HD21	1.94	0.49
1:C:305:LEU:HD23	1:C:374:PHE:HZ	1.77	0.49
1:C:470:SER:HB3	1:C:473:VAL:CG1	2.42	0.49
1:A:576:VAL:O	1:A:580:GLN:HG2	2.13	0.49
2:D:34:MET:HE2	2:D:72:ARG:NH2	2.27	0.49
1:A:94:GLN:CD	1:A:94:GLN:H	2.12	0.49
2:B:76:LYS:O	2:B:77:ASN:HB2	2.11	0.49
1:C:7:VAL:HG13	1:C:66:LEU:CD2	2.43	0.49
1:C:570:GLU:O	1:C:574:LYS:HE2	2.13	0.49
2:B:36:TRP:NE1	2:B:81:LEU:HB2	2.27	0.49
2:D:74:ASN:O	2:D:77:ASN:ND2	2.45	0.49
2:B:47:GLY:O	2:B:61:ALA:HB2	2.12	0.49
1:C:31:LEU:HB2	1:C:39:HIS:HE1	1.77	0.48
2:D:11:LEU:HD23	2:D:12:VAL:N	2.28	0.48
2:B:36:TRP:HD1	2:B:70:ILE:HD12	1.77	0.48
1:C:249:ASP:CB	1:C:252:GLU:HG3	2.43	0.48
1:C:419:SER:O	1:C:423:LEU:HD12	2.12	0.48
1:C:42:LEU:HD21	1:C:77:VAL:HG21	1.94	0.48
1:C:377:PHE:O	1:C:381:VAL:HG23	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:529:LEU:O	1:C:533:VAL:HG23	2.14	0.48
1:A:475:LYS:O	1:A:479:GLU:HG2	2.13	0.48
1:C:415:VAL:HG23	1:C:418:VAL:HG12	1.96	0.48
1:C:418:VAL:HG13	1:C:423:LEU:CD1	2.33	0.48
2:D:22:CYS:CB	2:D:96:CYS:HG	2.21	0.48
1:A:76:THR:O	1:A:77:VAL:HB	2.12	0.48
1:C:208:GLU:HG2	1:C:239:THR:HG21	1.95	0.48
1:C:462:VAL:O	1:C:465:GLU:HG3	2.14	0.48
1:C:433:VAL:O	1:C:436:LYS:O	2.31	0.48
2:D:40:PRO:HB2	2:D:43:LYS:HE2	1.95	0.48
2:D:71:SER:O	2:D:79:LEU:HD12	2.14	0.48
1:A:473:VAL:O	1:A:477:CYS:SG	2.72	0.47
2:B:47:GLY:HA3	2:B:104:MET:CE	2.44	0.47
1:C:90:CYS:SG	1:C:101:CYS:SG	3.12	0.47
1:A:404:GLN:O	1:A:408:LEU:CD1	2.62	0.47
1:C:338:HIS:ND1	1:C:341:TYR:CZ	2.82	0.47
1:C:580:GLN:O	1:C:583:LEU:HG	2.13	0.47
1:A:103:LEU:O	1:A:104:GLN:CG	2.63	0.47
1:A:543:GLN:O	1:A:546:ALA:HB3	2.15	0.47
1:C:481:LEU:HG	1:C:482:VAL:H	1.80	0.47
1:C:446:MET:HB3	1:C:447:PRO:HD3	1.95	0.47
1:A:354:GLU:HG2	1:A:355:THR:N	2.30	0.47
2:B:73:ASP:CB	2:B:76:LYS:HB2	2.43	0.47
1:C:516:LEU:O	1:C:521:ARG:NH2	2.47	0.47
1:A:417:GLN:NE2	1:A:494:ASP:OD2	2.37	0.47
1:A:356:THR:HG21	1:A:373:VAL:HG23	1.96	0.46
1:A:408:LEU:HD12	1:A:427:SER:CB	2.44	0.46
1:A:452:TYR:O	1:A:455:VAL:HG22	2.15	0.46
1:C:138:TYR:O	1:C:139:LEU:C	2.53	0.46
1:A:106:LYS:NZ	1:A:147:PRO:HB2	2.31	0.46
1:A:485:ARG:N	1:A:486:PRO:CD	2.78	0.46
1:C:344:VAL:O	1:C:348:ARG:HG3	2.15	0.46
2:B:22:CYS:HG	2:B:96:CYS:CB	2.27	0.46
1:A:529:LEU:O	1:A:533:VAL:HG23	2.16	0.46
1:C:97:GLU:CD	1:C:97:GLU:H	2.18	0.46
1:C:423:LEU:HD12	1:C:423:LEU:H	1.79	0.46
2:D:3:GLN:HG2	2:D:25:SER:HB2	1.98	0.46
1:A:10:ARG:NH1	1:A:255:ASP:OD2	2.48	0.45
1:A:31:LEU:CD2	1:A:74:LEU:HD22	2.47	0.45
1:A:453:LEU:O	1:A:457:LEU:HG	2.16	0.45
2:B:30:SER:O	2:B:72:ARG:NH2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:GLU:O	1:C:104:GLN:HB2	2.16	0.45
1:C:357:LEU:O	1:C:361:CYS:HB2	2.17	0.45
1:C:113:PRO:O	1:C:114:ARG:C	2.55	0.45
1:A:89:ASP:O	1:A:90:CYS:C	2.54	0.45
1:A:408:LEU:HD23	1:A:530:VAL:HG23	1.98	0.45
2:D:51:ILE:HD11	2:D:55:GLY:HA2	1.97	0.45
1:A:523:ILE:O	1:A:527:THR:OG1	2.23	0.45
1:A:33:GLN:HG2	1:A:112:LEU:HD21	1.99	0.45
1:A:87:MET:HE3	1:A:87:MET:HB2	1.89	0.45
1:A:121:ASP:OD1	1:A:121:ASP:N	2.49	0.45
1:A:186:ARG:HG3	1:A:190:LYS:HE2	1.98	0.45
1:A:494:ASP:OD1	1:A:496:THR:HG22	2.17	0.45
1:A:578:ALA:O	1:A:581:ALA:HB3	2.16	0.45
1:C:367:HIS:HA	1:C:370:TYR:CZ	2.52	0.45
1:C:302:LEU:HD12	1:C:302:LEU:HA	1.76	0.45
1:A:164:ALA:HB1	1:A:181:LYS:HD3	1.99	0.44
1:C:140:TYR:O	1:C:144:ARG:HB2	2.18	0.44
1:C:441:PRO:HG2	1:C:444:LYS:HG3	1.98	0.44
1:C:466:LYS:HE3	1:C:466:LYS:HB3	1.65	0.44
1:C:518:GLU:O	1:C:522:GLN:HG3	2.18	0.44
1:A:29:GLN:O	1:A:106:LYS:NZ	2.51	0.44
1:C:151:ALA:HB3	1:C:152:PRO:HD3	2.00	0.44
1:C:536:LYS:HZ3	1:C:583:LEU:HB3	1.82	0.44
1:C:521:ARG:HG2	1:C:525:LYS:HE2	2.00	0.44
1:A:352:THR:O	1:A:356:THR:HG23	2.17	0.44
1:A:408:LEU:CD1	1:A:427:SER:CB	2.96	0.44
1:C:3:HIS:O	1:C:3:HIS:CD2	2.70	0.44
1:C:249:ASP:HB3	1:C:252:GLU:CG	2.47	0.44
1:C:73:LYS:O	1:C:76:THR:OG1	2.27	0.44
1:C:475:LYS:O	1:C:476:CYS:C	2.55	0.44
2:D:45:LEU:HD13	2:D:45:LEU:HA	1.90	0.44
1:A:452:TYR:O	1:A:456:VAL:HG23	2.17	0.43
1:C:502:PHE:O	1:C:503:ASN:C	2.56	0.43
1:C:5:SER:OG	1:C:7:VAL:HG23	2.19	0.43
1:C:31:LEU:HB2	1:C:39:HIS:CE1	2.53	0.43
1:C:206:PHE:CZ	1:C:480:SER:HA	2.54	0.43
1:A:151:ALA:N	1:A:152:PRO:CD	2.81	0.43
1:A:479:GLU:OE1	1:A:479:GLU:HA	2.18	0.43
1:C:96:PRO:HD2	1:C:97:GLU:CD	2.39	0.43
1:C:530:VAL:CG1	1:C:534:LYS:HE3	2.49	0.43
1:A:408:LEU:HD23	1:A:530:VAL:CG2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:TYR:CZ	1:A:165:PHE:HE2	2.36	0.43
1:C:23:VAL:HG23	1:C:43:VAL:HG22	1.99	0.43
2:B:22:CYS:O	2:B:78:THR:HA	2.19	0.43
1:A:260:LEU:HD23	1:A:260:LEU:HA	1.88	0.43
1:A:356:THR:O	1:A:359:LYS:HG3	2.19	0.43
2:B:51:ILE:CD1	2:B:55:GLY:HA2	2.48	0.43
1:C:135:LEU:O	1:C:138:TYR:HB3	2.18	0.43
1:C:554:PHE:HE1	1:C:572:GLY:N	2.17	0.43
1:A:154:LEU:HD12	1:A:154:LEU:HA	1.84	0.42
1:A:22:LEU:CD1	1:A:151:ALA:HB1	2.49	0.42
1:A:22:LEU:HD12	1:A:22:LEU:HA	1.83	0.42
1:A:141:GLU:O	1:A:145:ARG:HG3	2.19	0.42
1:A:154:LEU:O	1:A:155:LEU:C	2.56	0.42
1:A:415:VAL:HG23	1:A:415:VAL:O	2.19	0.42
1:C:29:GLN:HE21	1:C:147:PRO:HA	1.83	0.42
1:C:99:ASN:HD22	1:C:99:ASN:HA	1.65	0.42
1:C:119:GLU:HB2	1:C:122:VAL:HG23	2.01	0.42
1:A:344:VAL:O	1:A:348:ARG:HG3	2.18	0.42
2:B:51:ILE:HD12	2:B:58:THR:HG22	2.02	0.42
1:A:34:CYS:HA	1:A:35:PRO:HD3	1.94	0.42
1:C:34:CYS:HA	1:C:35:PRO:HD3	1.87	0.42
1:C:483:ASN:O	1:C:487:CYS:HB2	2.19	0.42
1:C:485:ARG:HB3	1:C:486:PRO:HD3	2.00	0.42
1:A:93:LYS:HZ3	1:A:93:LYS:HG3	1.69	0.42
1:C:367:HIS:HA	1:C:370:TYR:CE1	2.54	0.42
2:B:110:ARG:HD3	2:B:111:TYR:CZ	2.55	0.42
1:C:91:CYS:O	1:C:92:ALA:C	2.57	0.42
1:A:244:GLU:O	1:A:248:GLY:N	2.42	0.42
1:A:103:LEU:C	1:A:105:HIS:H	2.23	0.42
1:A:360:CYS:O	1:A:363:ALA:HB3	2.20	0.42
1:A:179:LEU:HB3	1:A:182:LEU:HG	2.02	0.41
1:A:420:THR:HA	1:A:423:LEU:HD13	2.00	0.41
2:B:87:LYS:HA	2:B:87:LYS:HE3	2.02	0.41
1:A:306:ALA:O	1:A:310:VAL:N	2.48	0.41
1:C:151:ALA:HB2	1:C:250:LEU:HG	2.02	0.41
1:C:470:SER:O	1:C:473:VAL:HG13	2.19	0.41
1:A:60:GLU:H	1:A:60:GLU:HG3	1.62	0.41
1:A:95:GLU:OE1	1:A:101:CYS:HB3	2.20	0.41
1:A:249:ASP:OD1	1:A:249:ASP:N	2.51	0.41
1:A:340:ASP:O	1:A:447:PRO:HD3	2.20	0.41
1:C:500:LYS:HB2	1:C:500:LYS:HE2	1.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:LEU:HD23	1:C:260:LEU:HA	1.83	0.41
1:A:154:LEU:C	1:A:156:PHE:N	2.73	0.41
1:A:416:PRO:HB2	1:A:497:TYR:CE1	2.56	0.41
1:A:227:GLU:HG2	1:A:230:GLU:HB2	2.02	0.41
1:A:95:GLU:OE2	1:A:95:GLU:N	2.53	0.41
1:A:148:TYR:CD2	1:A:197:ARG:HD3	2.56	0.41
1:A:211:PHE:CD1	1:A:239:THR:HG23	2.56	0.41
1:C:308:ASP:OD2	2:D:52:SER:HB2	2.21	0.41
1:C:415:VAL:HG23	1:C:418:VAL:HG11	2.02	0.41
1:A:115:LEU:HD12	1:A:115:LEU:HA	1.77	0.40
1:C:99:ASN:O	1:C:100:GLU:C	2.58	0.40
1:C:204:GLN:HE21	1:C:204:GLN:HB2	1.69	0.40
1:A:95:GLU:HA	1:A:96:PRO:HD3	1.88	0.40
1:A:471:ASP:OD1	1:A:471:ASP:N	2.53	0.40
1:A:179:LEU:HD22	1:A:182:LEU:HG	2.04	0.40
2:D:40:PRO:HA	2:D:41:PRO:HD3	1.97	0.40
1:A:117:ARG:HA	1:A:118:PRO:HD3	1.81	0.40
1:A:141:GLU:OE1	1:A:145:ARG:NH1	2.48	0.40
1:A:63:ASP:OD1	1:A:63:ASP:N	2.54	0.40
1:A:230:GLU:OE2	1:A:263:TYR:OH	2.21	0.40
1:A:395:PHE:CE2	1:A:435:SER:HB3	2.56	0.40
1:C:156:PHE:O	1:C:159:LYS:N	2.54	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:93:ARG:NH2	1:C:56:ASP:OD2[2_546]	1.49	0.71
1:A:119:GLU:OE2	1:C:77:VAL:O[1_554]	2.12	0.08

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	554/591 (94%)	528 (95%)	26 (5%)	0	100	100
1	C	564/591 (95%)	535 (95%)	29 (5%)	0	100	100
2	B	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
2	D	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
All	All	1358/1426 (95%)	1290 (95%)	68 (5%)	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	500/516 (97%)	455 (91%)	45 (9%)	8	23
1	C	502/516 (97%)	435 (87%)	67 (13%)	3	9
2	B	97/97 (100%)	91 (94%)	6 (6%)	15	39
2	D	97/97 (100%)	91 (94%)	6 (6%)	15	39
All	All	1196/1226 (98%)	1072 (90%)	124 (10%)	5	16

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	GLU
1	A	19	PHE
1	A	22	LEU
1	A	24	LEU
1	A	31	LEU
1	A	34	CYS
1	A	87	MET
1	A	89	ASP
1	A	91	CYS
1	A	93	LYS
1	A	94	GLN
1	A	103	LEU
1	A	105	HIS

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Mol	Chain	Res	Type
1	A	107	ASP
1	A	121	ASP
1	A	130	ASN
1	A	132	GLU
1	A	147	PRO
1	A	149	PHE
1	A	153	GLU
1	A	166	THR
1	A	204	GLN
1	A	249	ASP
1	A	250	LEU
1	A	284	LEU
1	A	286	LYS
1	A	287	SER
1	A	289	CYS
1	A	305	LEU
1	A	317	LYS
1	A	334	TYR
1	A	344	VAL
1	A	354	GLU
1	A	365	ASP
1	A	370	TYR
1	A	389	LYS
1	A	412	THR
1	A	453	LEU
1	A	469	VAL
1	A	471	ASP
1	A	481	LEU
1	A	484	ARG
1	A	486	PRO
1	A	515	THR
1	A	538	LYS
2	B	12	VAL
2	B	25	SER
2	B	72	ARG
2	B	87	LYS
2	B	103	THR
2	B	122	SER
1	C	4	LYS
1	C	7	VAL
1	C	34	CYS
1	C	60	GLU

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Mol	Chain	Res	Type
1	C	65	SER
1	C	72	ASP
1	C	73	LYS
1	C	89	ASP
1	C	91	CYS
1	C	93	LYS
1	C	94	GLN
1	C	95	GLU
1	C	97	GLU
1	C	99	ASN
1	C	101	CYS
1	C	104	GLN
1	C	107	ASP
1	C	108	ASP
1	C	109	ASN
1	C	114	ARG
1	C	115	LEU
1	C	116	VAL
1	C	132	GLU
1	C	137	LYS
1	C	147	PRO
1	C	149	PHE
1	C	166	THR
1	C	174	LYS
1	C	179	LEU
1	C	198	LEU
1	C	203	LEU
1	C	232	SER
1	C	233	LYS
1	C	252	GLU
1	C	283	LEU
1	C	287	SER
1	C	302	LEU
1	C	304	SER
1	C	334	TYR
1	C	344	VAL
1	C	356	THR
1	C	365	ASP
1	C	368	GLU
1	C	370	TYR
1	C	419	SER
1	C	427	SER

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Mol	Chain	Res	Type
1	C	435	SER
1	C	436	LYS
1	C	439	LYS
1	C	447	PRO
1	C	450	GLU
1	C	453	LEU
1	C	465	GLU
1	C	466	LYS
1	C	471	ASP
1	C	473	VAL
1	C	475	LYS
1	C	480	SER
1	C	481	LEU
1	C	498	VAL
1	C	500	LYS
1	C	501	GLU
1	C	518	GLU
1	C	519	LYS
1	C	544	LEU
1	C	548	MET
1	C	574	LYS
2	D	1	GLU
2	D	12	VAL
2	D	29	SER
2	D	31	THR
2	D	103	THR
2	D	122	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	32	GLN
1	A	146	HIS
2	B	77	ASN
2	B	82	GLN
1	C	3	HIS
1	C	9	HIS
1	C	18	ASN
1	C	29	GLN
1	C	94	GLN
1	C	105	HIS

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Mol	Chain	Res	Type
1	C	204	GLN
1	C	535	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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

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, 95^{th} 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	567/591 (95%)	0.32	26 (4%)	38	33	41, 72, 110, 178	1 (0%)
1	C	571/591 (96%)	0.28	27 (4%)	37	32	41, 69, 106, 176	1 (0%)
2	B	122/122 (100%)	-0.03	1 (0%)	82	79	43, 60, 75, 127	0
2	D	122/122 (100%)	-0.09	2 (1%)	70	65	48, 62, 80, 127	0
All	All	1382/1426 (96%)	0.24	56 (4%)	42	36	41, 69, 106, 178	2 (0%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	80	LEU	5.5
1	A	176	ALA	4.7
1	A	94	GLN	4.6
1	C	169	CYS	4.4
1	C	95	GLU	4.4
1	C	176	ALA	4.3
1	A	95	GLU	4.0
1	C	94	GLN	3.9
1	A	96	PRO	3.7
1	A	177	CYS	3.5
1	A	80	LEU	3.4
1	A	179	LEU	3.4
1	C	93	LYS	3.4
2	B	2	VAL	3.3
1	C	584	GLY	3.3
1	C	91	CYS	3.3
1	C	396	GLU	3.2
1	A	93	LYS	3.1
1	C	437	CYS	3.1
1	A	250	LEU	2.9
1	C	79	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	97	GLU	2.9
1	C	76	THR	2.8
1	A	513	ILE	2.8
2	D	1	GLU	2.7
2	D	2	VAL	2.7
1	C	96	PRO	2.7
1	C	61	ASN	2.7
1	A	87	MET	2.7
1	A	111	ASN	2.6
1	A	106	LYS	2.5
1	C	360	CYS	2.5
1	A	105	HIS	2.5
1	C	77	VAL	2.4
1	A	548	MET	2.4
1	A	91	CYS	2.4
1	A	461	CYS	2.4
1	C	418	VAL	2.3
1	C	90	CYS	2.3
1	C	583	LEU	2.3
1	A	61	ASN	2.3
1	A	19	PHE	2.3
1	C	175	ALA	2.3
1	A	76	THR	2.2
1	C	113	PRO	2.2
1	A	99	ASN	2.2
1	A	63	ASP	2.2
1	C	107	ASP	2.2
1	C	174	LYS	2.1
1	A	3	HIS	2.1
1	C	99	ASN	2.1
1	A	169	CYS	2.1
1	C	253	CYS	2.1
1	A	138	TYR	2.0
1	A	102	PHE	2.0
1	C	457	LEU	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 monosaccharides 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.