



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:46 AM UTC

PDB ID : 4WKG / pdb_00004wkg
Title : The crystal structure of apo ArnA features an unexpected central binding pocket and provides an explanation for enzymatic coop-erativity
Authors : Grimm, C.
Deposited on : 2014-10-02
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

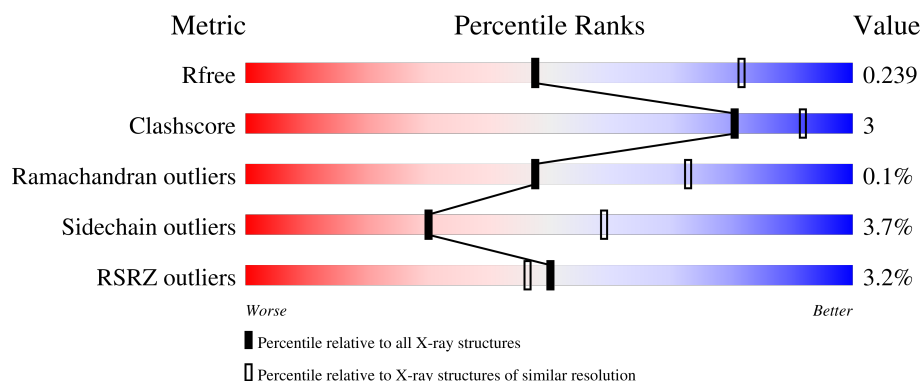
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

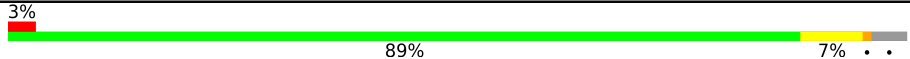
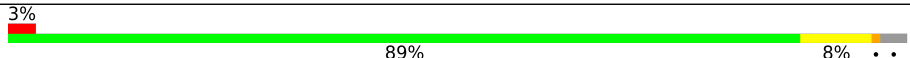
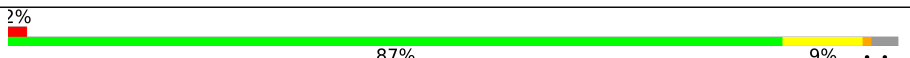
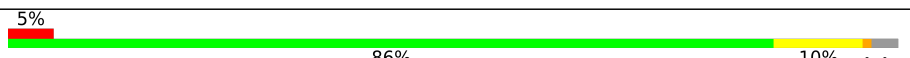
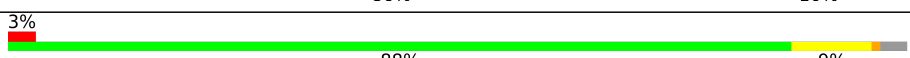
The reported resolution of this entry is 2.70 Å.

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.



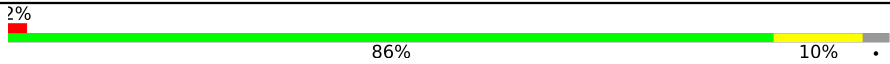
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	660	
1	B	660	
1	C	660	
1	D	660	
1	E	660	

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Mol	Chain	Length	Quality of chain
1	F	660	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: a small red segment at the beginning labeled '2%', a large green segment labeled '86%', a small yellow segment labeled '10%', and a very small grey segment at the end. A small black dot is located at the far right end of the bar.

2 Entry composition [i](#)

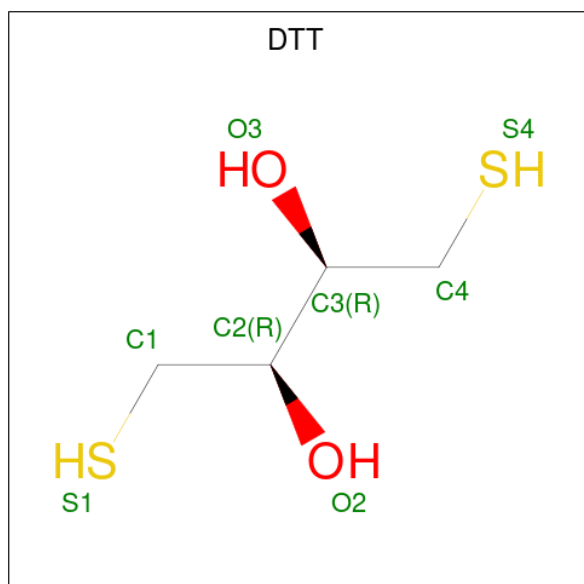
There are 4 unique types of molecules in this entry. The entry contains 60000 atoms, of which 29761 are hydrogens and 0 are deuteriums.

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 Bifunctional polymyxin resistance protein ArnA.

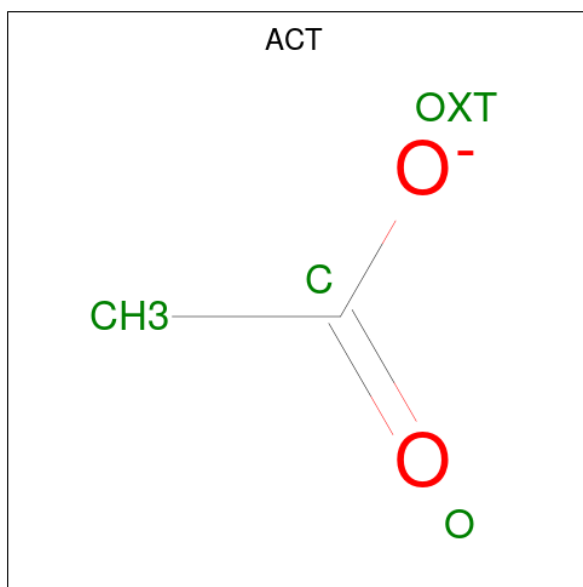
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	636	Total	C	H	N	O	S	0	0	0
			9951	3195	4945	889	903	19			
1	B	643	Total	C	H	N	O	S	0	0	0
			10036	3234	4972	897	914	19			
1	C	637	Total	C	H	N	O	S	0	0	0
			9963	3203	4947	888	906	19			
1	D	641	Total	C	H	N	O	S	0	0	0
			9973	3218	4936	889	911	19			
1	E	643	Total	C	H	N	O	S	0	0	0
			10032	3231	4974	894	914	19			
1	F	637	Total	C	H	N	O	S	0	0	0
			9950	3197	4941	888	905	19			

- Molecule 2 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (CCD ID: DTT) (formula: C₄H₁₀O₂S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	O	S	0	1
			36	8	20	4	4		
2	D	1	Total	C	H	O	S	0	1
			36	8	20	4	4		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			7	2	3	2		
3	F	1	Total	C	H	O	0	0
			7	2	3	2		

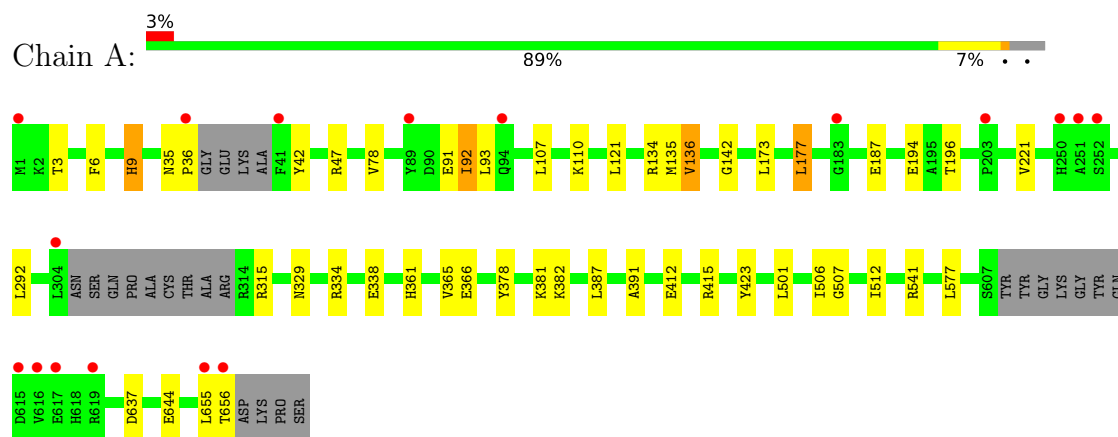
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	B	2	Total	O	0	0
			2	2		
4	C	2	Total	O	0	0
			2	2		
4	D	1	Total	O	0	0
			1	1		
4	E	2	Total	O	0	0
			2	2		
4	F	1	Total	O	0	0
			1	1		

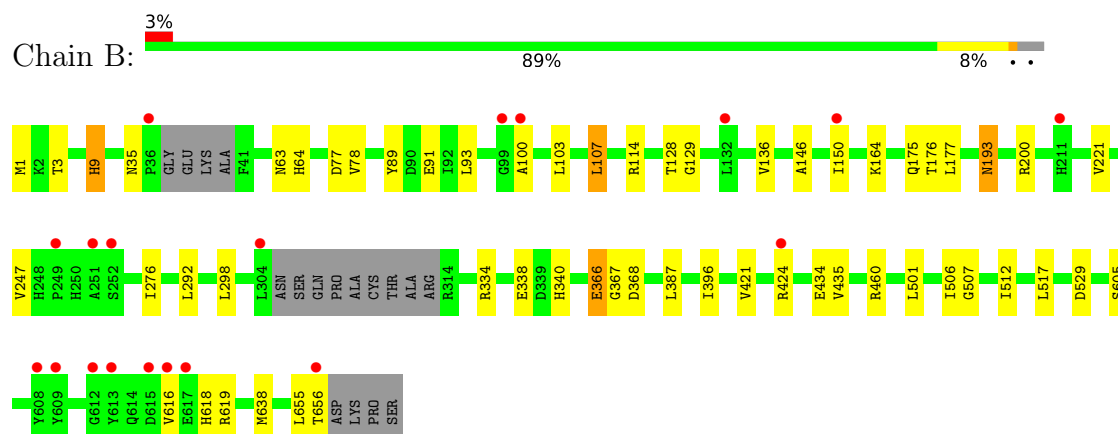
3 Residue-property plots [i](#)

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.

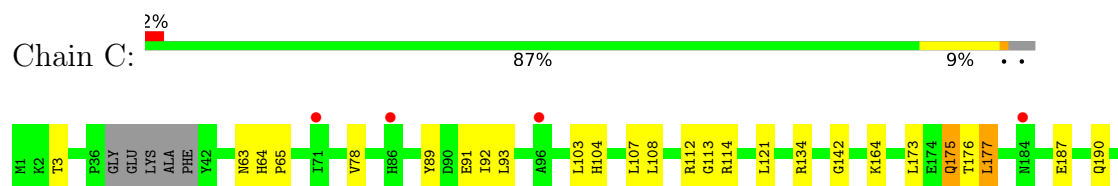
- Molecule 1: Bifunctional polymyxin resistance protein ArnA

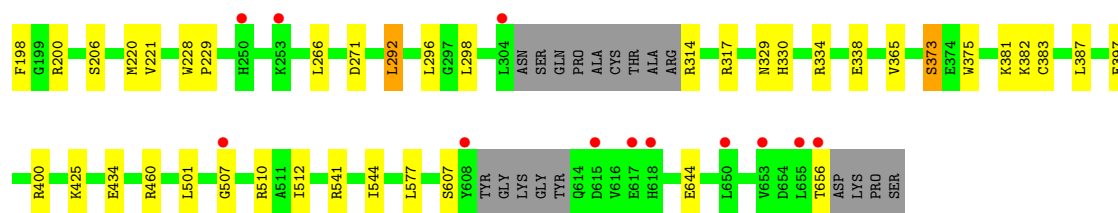


- Molecule 1: Bifunctional polymyxin resistance protein ArnA

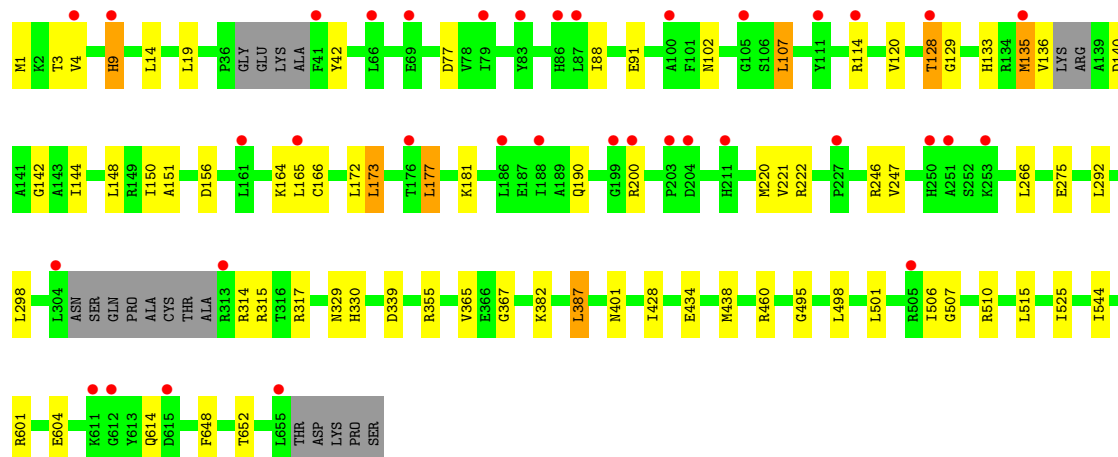
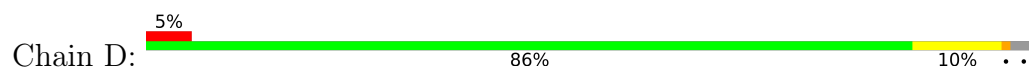


- Molecule 1: Bifunctional polymyxin resistance protein ArnA

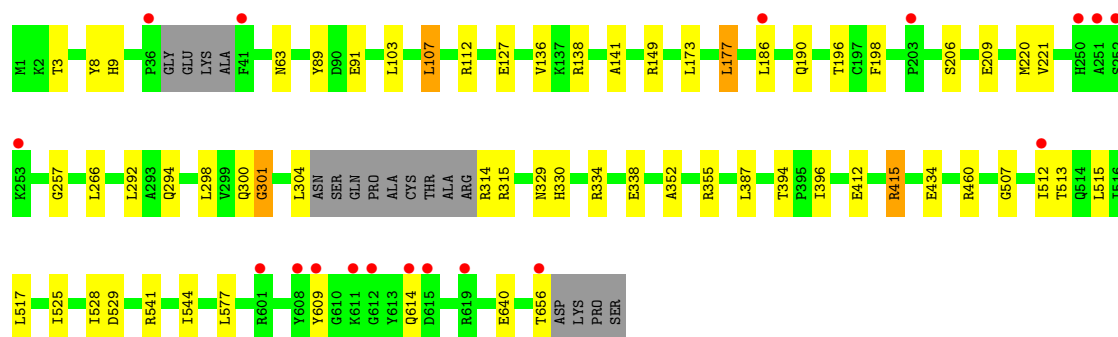
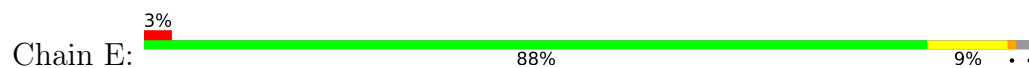




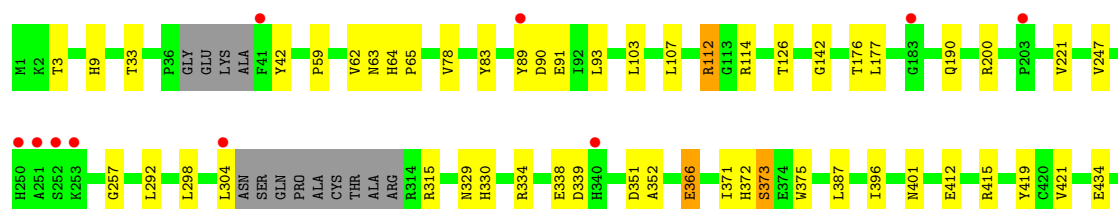
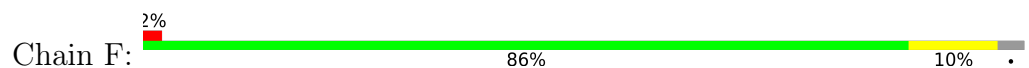
• Molecule 1: Bifunctional polymyxin resistance protein ArnA



• Molecule 1: Bifunctional polymyxin resistance protein ArnA



• Molecule 1: Bifunctional polymyxin resistance protein ArnA





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	106.72Å 112.82Å 113.61Å 81.92° 82.96° 83.80°	Depositor
Resolution (Å)	48.16 – 2.70 48.16 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.4 (48.16-2.70) 90.0 (48.16-2.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.205 , 0.232 0.215 , 0.239	Depositor DCC
R_{free} test set	6967 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	69.0	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 33.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.014 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	60000	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, DTT

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	0.39	0/5126	0.75	1/6965 (0.0%)
1	B	0.40	0/5188	0.78	5/7051 (0.1%)
1	C	0.38	0/5137	0.75	2/6981 (0.0%)
1	D	0.40	0/5160	0.79	5/7013 (0.1%)
1	E	0.39	0/5182	0.78	3/7044 (0.0%)
1	F	0.39	0/5129	0.76	0/6970
All	All	0.39	0/30922	0.77	16/42024 (0.0%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	507	GLY	N-CA-C	12.05	126.47	113.58
1	C	507	GLY	N-CA-C	11.47	125.85	113.58
1	D	507	GLY	N-CA-C	10.84	125.17	113.58
1	A	507	GLY	N-CA-C	10.60	124.92	113.58
1	E	301	GLY	CA-C-N	9.11	137.98	121.85
1	E	301	GLY	C-N-CA	9.11	137.98	121.85
1	D	506	ILE	N-CA-C	6.39	118.37	109.55
1	D	135	MET	CB-CA-C	-6.25	109.38	116.63
1	B	507	GLY	N-CA-C	6.16	127.77	113.18
1	B	506	ILE	N-CA-C	5.77	117.52	109.55
1	D	88	ILE	N-CA-C	5.70	116.51	108.36
1	B	9	HIS	CB-CA-C	-5.36	108.81	115.89
1	B	367	GLY	N-CA-C	5.34	118.28	110.38
1	C	607	SER	N-CA-C	-5.32	105.37	111.07
1	D	367	GLY	N-CA-C	5.09	117.91	110.38
1	B	340	HIS	N-CA-C	5.04	119.12	112.92

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	5006	4945	4933	22	0
1	B	5064	4972	4977	25	0
1	C	5016	4947	4937	28	0
1	D	5037	4936	4936	34	0
1	E	5058	4974	4966	26	0
1	F	5009	4941	4930	29	0
2	A	16	20	20	0	0
2	D	16	20	20	1	0
3	A	4	3	3	0	0
3	F	4	3	3	1	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	1	0	0	0	0
4	E	2	0	0	0	0
4	F	1	0	0	0	0
All	All	30239	29761	29725	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 3.

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:D:434:GLU:OE1	1:D:460:ARG:NH2	2.16	0.77
1:A:382:LYS:NZ	1:B:366:GLU:OE2	2.19	0.76
1:B:434:GLU:HG2	1:B:619:ARG:HH22	1.50	0.75
1:F:500:ASN:ND2	1:F:502:ASN:OD1	2.21	0.74
1:F:415:ARG:NH2	1:F:419:TYR:OH	2.21	0.73
1:F:434:GLU:OE1	1:F:460:ARG:NH2	2.22	0.73
1:D:329:ASN:OD1	1:D:355:ARG:NH2	2.21	0.73
1:A:381:LYS:NZ	1:B:368:ASP:OD2	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:412:GLU:OE1	1:E:415:ARG:NH1	2.23	0.71
1:D:151:ALA:O	1:D:164:LYS:NZ	2.19	0.68
1:F:329:ASN:ND2	1:F:352:ALA:O	2.26	0.67
1:C:383:CYS:O	1:C:425:LYS:NZ	2.25	0.65
1:A:541:ARG:NH2	1:A:644:GLU:OE1	2.28	0.65
1:A:655:LEU:O	1:A:656:THR:OG1	2.08	0.65
1:C:381:LYS:O	1:C:425:LYS:NZ	2.29	0.63
1:C:334:ARG:NH1	1:C:338:GLU:OE2	2.33	0.61
1:D:128:THR:OG1	1:D:129:GLY:N	2.34	0.60
1:F:529:ASP:OD2	1:F:605:SER:OG	2.18	0.60
1:B:334:ARG:NH1	1:B:338:GLU:OE2	2.35	0.59
1:B:529:ASP:OD2	1:B:605:SER:OG	2.20	0.59
1:C:134:ARG:NH2	1:C:187:GLU:OE2	2.36	0.58
1:D:501:LEU:O	1:D:510:ARG:NH1	2.33	0.58
1:F:351:ASP:OD1	1:F:352:ALA:N	2.38	0.57
1:B:434:GLU:OE1	1:B:460:ARG:NH2	2.39	0.56
1:F:112:ARG:NH1	1:F:190:GLN:OE1	2.38	0.56
1:D:107:LEU:HD13	1:D:129:GLY:HA3	1.89	0.55
1:D:102:ASN:HB2	1:D:135:MET:SD	2.47	0.55
1:E:512:ILE:HG22	1:E:577:LEU:HD21	1.89	0.55
1:F:64:HIS:HD2	1:F:65:PRO:HD2	1.71	0.55
1:A:3:THR:HG22	1:A:78:VAL:HG13	1.89	0.54
1:C:206:SER:HA	1:C:220:MET:HE2	1.89	0.54
1:C:501:LEU:O	1:C:510:ARG:NH1	2.37	0.54
1:F:3:THR:HG22	1:F:78:VAL:HG13	1.88	0.54
1:E:541:ARG:NH1	1:E:640:GLU:OE2	2.41	0.53
1:D:135:MET:O	1:D:136:VAL:HG22	2.08	0.53
1:C:373:SER:HB3	1:C:375:TRP:CZ3	2.44	0.53
1:E:334:ARG:NH1	1:E:338:GLU:OE2	2.41	0.52
1:C:434:GLU:OE1	1:C:460:ARG:NH2	2.43	0.52
1:F:512:ILE:HG22	1:F:577:LEU:HD21	1.92	0.52
1:C:3:THR:HG22	1:C:78:VAL:HG13	1.92	0.51
1:E:329:ASN:ND2	1:E:352:ALA:O	2.43	0.51
1:E:63:ASN:HB3	1:E:89:TYR:CZ	2.47	0.51
1:E:460:ARG:NH1	1:E:614:GLN:O	2.44	0.51
1:C:512:ILE:HG22	1:C:577:LEU:HD21	1.94	0.50
1:F:372:HIS:NE2	1:F:412:GLU:OE1	2.43	0.50
1:E:329:ASN:OD1	1:E:355:ARG:NH2	2.42	0.50
1:D:142:GLY:O	1:D:190:GLN:NE2	2.41	0.50
1:F:257:GLY:O	1:F:304:LEU:HD12	2.12	0.50
1:B:150:ILE:HD12	1:B:164:LYS:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:ASP:O	1:D:222:ARG:NH1	2.42	0.49
1:C:63:ASN:HB3	1:C:89:TYR:CZ	2.47	0.49
1:D:150:ILE:HD13	1:D:165:LEU:HD21	1.95	0.49
1:A:9:HIS:CE1	1:A:42:TYR:CB	2.96	0.48
1:A:378:TYR:OH	1:B:366:GLU:HG3	2.14	0.48
1:E:515:LEU:HD22	1:E:525:ILE:HG23	1.94	0.48
1:B:128:THR:O	1:B:150:ILE:HG22	2.14	0.47
1:B:3:THR:HG22	1:B:78:VAL:HG13	1.96	0.47
1:C:397:GLU:OE2	1:C:400:ARG:NH1	2.48	0.47
1:F:63:ASN:HB3	1:F:89:TYR:CZ	2.49	0.47
1:A:381:LYS:HD2	1:A:423:TYR:CE1	2.50	0.47
1:D:315:ARG:CZ	1:D:339:ASP:O	2.62	0.47
1:F:142:GLY:O	1:F:190:GLN:NE2	2.46	0.47
1:B:107:LEU:HD13	1:B:129:GLY:HA3	1.96	0.47
1:F:114:ARG:HD2	1:F:200:ARG:CB	2.45	0.47
1:A:173:LEU:O	1:A:177:LEU:HB2	2.15	0.47
1:A:512:ILE:HD11	1:A:577:LEU:HD11	1.96	0.47
1:D:330:HIS:HB3	1:D:544:ILE:HG13	1.96	0.46
1:D:382:LYS:NZ	1:F:366:GLU:OE1	2.42	0.46
1:D:495:GLY:O	1:D:498:LEU:CD1	2.63	0.46
1:B:150:ILE:CD1	1:B:164:LYS:HB3	2.45	0.46
1:C:541:ARG:NH2	1:C:644:GLU:OE2	2.48	0.46
1:F:83:TYR:OH	3:F:701:ACT:H3	2.15	0.46
1:C:114:ARG:HD2	1:C:200:ARG:HA	1.98	0.46
1:D:120:VAL:HG21	1:D:128:THR:HG21	1.98	0.46
1:D:133:HIS:NE2	1:D:140:ASP:HA	2.30	0.46
1:B:63:ASN:HB3	1:B:89:TYR:CZ	2.50	0.46
1:C:64:HIS:HD2	1:C:65:PRO:HD2	1.81	0.46
1:F:330:HIS:HB3	1:F:544:ILE:HG13	1.98	0.46
1:B:193:ASN:OD1	1:B:193:ASN:N	2.48	0.45
1:D:601:ARG:NH2	1:E:294:GLN:HB3	2.30	0.45
1:E:528:ILE:HD13	1:E:609:TYR:CE2	2.51	0.45
1:F:9:HIS:CD2	1:F:42:TYR:CB	2.99	0.45
1:A:334:ARG:NH1	1:A:338:GLU:OE2	2.49	0.45
1:E:107:LEU:HD21	1:E:149:ARG:HG2	1.97	0.45
1:A:315:ARG:CZ	1:A:361:HIS:CE1	3.00	0.45
1:F:334:ARG:NH1	1:F:338:GLU:OE2	2.49	0.45
1:E:141:ALA:HA	1:E:190:GLN:HE22	1.82	0.45
1:B:64:HIS:NE2	1:E:529:ASP:OD1	2.50	0.45
1:C:114:ARG:HD2	1:C:200:ARG:CA	2.46	0.45
1:E:173:LEU:O	1:E:177:LEU:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:ILE:HG13	1:D:190:GLN:HG3	1.99	0.45
1:D:148:LEU:HB2	1:D:172:LEU:HD12	1.97	0.45
1:D:515:LEU:HD22	1:D:525:ILE:HG23	1.99	0.45
1:E:206:SER:HA	1:E:220:MET:HE2	1.98	0.45
1:A:135:MET:O	1:A:136:VAL:HG13	2.17	0.44
1:B:175:GLN:HG3	1:B:176:THR:HG23	1.99	0.44
1:B:421:VAL:O	1:B:424:ARG:NH1	2.49	0.44
1:A:35:ASN:CG	1:A:36:PRO:HD2	2.43	0.44
1:A:134:ARG:NH2	1:A:187:GLU:OE2	2.40	0.44
1:C:113:GLY:HA3	1:C:198:PHE:H	1.83	0.44
1:B:128:THR:C	1:B:150:ILE:HG22	2.42	0.44
1:B:655:LEU:O	1:B:656:THR:CB	2.66	0.44
1:F:512:ILE:HG13	1:F:513:THR:N	2.33	0.44
1:C:228:TRP:HB3	1:C:229:PRO:HD2	2.00	0.44
1:D:1:MET:SD	1:D:181:LYS:HA	2.57	0.44
1:D:314:ARG:NH2	1:D:317:ARG:CZ	2.81	0.43
1:A:412:GLU:OE1	1:A:415:ARG:NH1	2.44	0.43
1:C:175:GLN:HG2	1:C:176:THR:HG23	2.00	0.43
1:D:114:ARG:HD2	1:D:200:ARG:CB	2.49	0.43
1:C:112:ARG:NH2	1:C:190:GLN:OE1	2.51	0.43
1:E:394:THR:HG22	1:E:396:ILE:HG22	1.99	0.43
1:C:134:ARG:O	1:C:142:GLY:HA3	2.18	0.43
1:A:391:ALA:HB3	1:A:506:ILE:HD11	2.01	0.43
1:C:330:HIS:HB3	1:C:544:ILE:HG13	2.00	0.43
1:B:1:MET:HE2	1:B:77:ASP:HB3	2.00	0.43
1:E:196:THR:CG2	1:E:198:PHE:CE1	3.02	0.43
1:C:314:ARG:NH2	1:C:317:ARG:CZ	2.81	0.42
1:D:19:LEU:HD13	1:D:177:LEU:HD21	2.01	0.42
1:E:127:GLU:OE2	1:E:149:ARG:NH1	2.52	0.42
1:C:64:HIS:CD2	1:C:65:PRO:HD2	2.54	0.42
1:D:438:MET:SD	1:D:614:GLN:NE2	2.93	0.42
1:E:330:HIS:HB3	1:E:544:ILE:HG13	2.01	0.42
1:F:315:ARG:NH2	1:F:339:ASP:O	2.53	0.42
1:A:134:ARG:O	1:A:142:GLY:HA3	2.20	0.42
1:C:104:HIS:CD2	1:C:108:LEU:HD21	2.55	0.42
1:D:387:LEU:HD12	1:D:428:ILE:HB	2.01	0.42
1:D:14:LEU:HD21	1:D:166:CYS:HA	2.01	0.42
1:C:173:LEU:O	1:C:177:LEU:HB2	2.19	0.42
1:B:93:LEU:HD12	1:B:100:ALA:HB3	2.02	0.41
1:E:434:GLU:OE1	1:E:460:ARG:NH2	2.53	0.41
1:E:138:ARG:HB2	1:E:141:ALA:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:90:ASP:HA	1:F:93:LEU:HB2	2.02	0.41
1:B:434:GLU:HG2	1:B:619:ARG:NH2	2.26	0.41
1:E:8:TYR:CE2	1:E:9:HIS:CE1	3.09	0.41
1:E:300:GLN:HA	1:E:301:GLY:HA2	1.90	0.41
1:F:549:ARG:NH1	1:F:631:ASP:O	2.50	0.41
1:A:6:PHE:CZ	1:A:92:ILE:HD11	2.56	0.41
1:A:381:LYS:HD2	1:A:423:TYR:CD1	2.54	0.41
1:D:246:ARG:HB3	1:D:275:GLU:HB3	2.02	0.41
1:B:146:ALA:CB	1:B:176:THR:HG21	2.50	0.41
1:E:512:ILE:HG13	1:E:513:THR:N	2.36	0.41
1:F:491:PHE:CZ	1:F:621:PRO:HB3	2.55	0.41
1:D:315:ARG:NH2	1:D:339:ASP:O	2.54	0.41
1:F:59:PRO:HG2	1:F:62:VAL:HG22	2.03	0.41
1:A:366:GLU:OE1	1:C:382:LYS:NZ	2.51	0.41
1:D:173:LEU:CD2	1:D:177:LEU:HD22	2.50	0.41
1:D:9:HIS:CE1	1:D:42:TYR:CB	3.05	0.41
1:E:257:GLY:O	1:E:304:LEU:HD12	2.21	0.41
1:B:616:VAL:HG21	1:B:619:ARG:HH21	1.86	0.40
1:F:373:SER:HB2	1:F:375:TRP:CD2	2.56	0.40
1:F:373:SER:HB3	1:F:375:TRP:CH2	2.56	0.40
1:B:114:ARG:HH11	1:B:200:ARG:HH11	1.70	0.40
1:A:110:LYS:NZ	1:A:194:GLU:O	2.54	0.40
1:D:648:PHE:O	1:D:652:THR:HG23	2.21	0.40
2:D:701[B]:DTT:H41	1:F:375:TRP:HB3	2.04	0.40
1:C:292:LEU:HD13	1:C:296:LEU:HD12	2.04	0.40
1:D:1:MET:HE2	1:D:77:ASP:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	628/660 (95%)	613 (98%)	14 (2%)	1 (0%)	43	68
1	B	637/660 (96%)	623 (98%)	13 (2%)	1 (0%)	43	68
1	C	629/660 (95%)	617 (98%)	12 (2%)	0	100	100
1	D	633/660 (96%)	619 (98%)	14 (2%)	0	100	100
1	E	637/660 (96%)	619 (97%)	17 (3%)	1 (0%)	43	68
1	F	629/660 (95%)	618 (98%)	11 (2%)	0	100	100
All	All	3793/3960 (96%)	3709 (98%)	81 (2%)	3 (0%)	48	73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	VAL
1	E	136	VAL
1	B	136	VAL

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	528/559 (94%)	512 (97%)	16 (3%)	36	66
1	B	532/559 (95%)	511 (96%)	21 (4%)	28	57
1	C	529/559 (95%)	510 (96%)	19 (4%)	31	60
1	D	528/559 (94%)	510 (97%)	18 (3%)	32	62
1	E	531/559 (95%)	513 (97%)	18 (3%)	32	62
1	F	528/559 (94%)	503 (95%)	25 (5%)	23	51
All	All	3176/3354 (95%)	3059 (96%)	117 (4%)	30	59

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	47	ARG

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Mol	Chain	Res	Type
1	A	91	GLU
1	A	92	ILE
1	A	93	LEU
1	A	107	LEU
1	A	121	LEU
1	A	177	LEU
1	A	196	THR
1	A	221	VAL
1	A	292	LEU
1	A	329	ASN
1	A	365	VAL
1	A	387	LEU
1	A	501	LEU
1	A	637	ASP
1	B	9	HIS
1	B	35	ASN
1	B	91	GLU
1	B	103	LEU
1	B	107	LEU
1	B	177	LEU
1	B	193	ASN
1	B	221	VAL
1	B	247	VAL
1	B	276	ILE
1	B	292	LEU
1	B	298	LEU
1	B	366	GLU
1	B	387	LEU
1	B	396	ILE
1	B	435	VAL
1	B	501	LEU
1	B	512	ILE
1	B	517	LEU
1	B	618	HIS
1	B	638	MET
1	C	91	GLU
1	C	92	ILE
1	C	93	LEU
1	C	103	LEU
1	C	107	LEU
1	C	121	LEU
1	C	164	LYS

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Mol	Chain	Res	Type
1	C	175	GLN
1	C	177	LEU
1	C	221	VAL
1	C	266	LEU
1	C	271	ASP
1	C	292	LEU
1	C	298	LEU
1	C	329	ASN
1	C	365	VAL
1	C	373	SER
1	C	387	LEU
1	C	656	THR
1	D	3	THR
1	D	4	VAL
1	D	9	HIS
1	D	91	GLU
1	D	107	LEU
1	D	128	THR
1	D	173	LEU
1	D	177	LEU
1	D	220	MET
1	D	221	VAL
1	D	247	VAL
1	D	266	LEU
1	D	292	LEU
1	D	298	LEU
1	D	365	VAL
1	D	387	LEU
1	D	401	ASN
1	D	604	GLU
1	E	3	THR
1	E	91	GLU
1	E	103	LEU
1	E	107	LEU
1	E	112	ARG
1	E	177	LEU
1	E	186	LEU
1	E	209	GLU
1	E	221	VAL
1	E	266	LEU
1	E	292	LEU
1	E	298	LEU

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Mol	Chain	Res	Type
1	E	314	ARG
1	E	315	ARG
1	E	387	LEU
1	E	415	ARG
1	E	517	LEU
1	E	656	THR
1	F	33	THR
1	F	91	GLU
1	F	103	LEU
1	F	107	LEU
1	F	112	ARG
1	F	126	THR
1	F	176	THR
1	F	177	LEU
1	F	221	VAL
1	F	247	VAL
1	F	292	LEU
1	F	298	LEU
1	F	366	GLU
1	F	371	ILE
1	F	373	SER
1	F	387	LEU
1	F	396	ILE
1	F	401	ASN
1	F	421	VAL
1	F	534	LYS
1	F	604	GLU
1	F	618	HIS
1	F	619	ARG
1	F	644	GLU
1	F	656	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	248	HIS
1	A	288	GLN
1	A	413	ASN
1	A	514	GLN
1	B	9	HIS
1	B	102	ASN
1	B	123	ASN

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Mol	Chain	Res	Type
1	B	379	HIS
1	B	518	ASN
1	B	588	HIS
1	C	64	HIS
1	C	102	ASN
1	C	167	HIS
1	C	218	HIS
1	C	413	ASN
1	C	514	GLN
1	C	518	ASN
1	C	614	GLN
1	D	104	HIS
1	D	518	ASN
1	D	556	ASN
1	E	102	ASN
1	E	190	GLN
1	E	372	HIS
1	F	9	HIS
1	F	64	HIS
1	F	118	ASN
1	F	218	HIS
1	F	248	HIS
1	F	329	ASN
1	F	518	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 ⓘ

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	DTT	A	701[A]	-	7,7,7	0.72	0	4,8,8	0.55	0
2	DTT	A	701[B]	-	7,7,7	0.61	0	4,8,8	0.31	0
3	ACT	A	702	-	3,3,3	0.79	0	3,3,3	1.41	0
2	DTT	D	701[A]	-	7,7,7	0.60	0	4,8,8	0.32	0
3	ACT	F	701	-	3,3,3	0.76	0	3,3,3	1.39	0
2	DTT	D	701[B]	-	7,7,7	0.57	0	4,8,8	0.27	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DTT	D	701[A]	-	-	1/8/8/8	-
2	DTT	A	701[A]	-	-	2/8/8/8	-
2	DTT	D	701[B]	-	-	1/8/8/8	-
2	DTT	A	701[B]	-	-	4/8/8/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701[A]	DTT	S1-C1-C2-O2
2	A	701[A]	DTT	S1-C1-C2-C3
2	A	701[B]	DTT	S1-C1-C2-O2
2	A	701[B]	DTT	S1-C1-C2-C3
2	A	701[B]	DTT	O3-C3-C4-S4
2	D	701[B]	DTT	S1-C1-C2-O2
2	A	701[B]	DTT	C2-C3-C4-S4
2	D	701[A]	DTT	C2-C3-C4-S4

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	701	ACT	1	0
2	D	701[B]	DTT	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	636/660 (96%)	-0.18	17 (2%) 56 53	22, 54, 98, 158	0
1	B	643/660 (97%)	-0.11	19 (2%) 52 49	23, 58, 108, 176	0
1	C	637/660 (96%)	-0.17	16 (2%) 58 55	31, 58, 103, 159	0
1	D	641/660 (97%)	0.19	36 (5%) 30 26	23, 73, 160, 209	0
1	E	643/660 (97%)	-0.23	18 (2%) 55 51	20, 52, 100, 157	0
1	F	637/660 (96%)	-0.08	15 (2%) 59 56	33, 63, 103, 156	0
All	All	3837/3960 (96%)	-0.10	121 (3%) 50 46	20, 59, 125, 209	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	100	ALA	5.4
1	D	79	ILE	5.4
1	D	313	ARG	5.0
1	D	304	LEU	4.2
1	E	41	PHE	4.1
1	C	608	TYR	4.1
1	F	252	SER	4.1
1	A	41	PHE	4.0
1	B	252	SER	4.0
1	D	655	LEU	4.0
1	B	617	GLU	3.9
1	F	41	PHE	3.8
1	C	656	THR	3.7
1	E	619	ARG	3.7
1	D	186	LEU	3.6
1	B	608	TYR	3.6
1	A	615	ASP	3.6
1	E	252	SER	3.5
1	D	87	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	615	ASP	3.5
1	D	41	PHE	3.5
1	D	204	ASP	3.4
1	B	100	ALA	3.3
1	F	537	PHE	3.3
1	F	615	ASP	3.3
1	E	203	PRO	3.3
1	F	203	PRO	3.3
1	B	251	ALA	3.2
1	C	615	ASP	3.2
1	C	655	LEU	3.2
1	A	251	ALA	3.2
1	E	251	ALA	3.1
1	A	252	SER	3.1
1	A	656	THR	3.0
1	A	250	HIS	3.0
1	B	656	THR	3.0
1	D	203	PRO	3.0
1	B	304	LEU	2.9
1	B	424	ARG	2.9
1	D	251	ALA	2.9
1	A	304	LEU	2.9
1	E	609	TYR	2.9
1	D	161	LEU	2.9
1	B	211	HIS	2.9
1	D	9	HIS	2.9
1	D	86	HIS	2.9
1	E	612	GLY	2.9
1	A	617	GLU	2.8
1	A	203	PRO	2.8
1	D	105	GLY	2.8
1	E	611	LYS	2.8
1	A	655	LEU	2.8
1	D	165	LEU	2.7
1	F	251	ALA	2.7
1	E	608	TYR	2.7
1	F	630	LEU	2.7
1	C	304	LEU	2.6
1	D	114	ARG	2.6
1	D	188	ILE	2.6
1	E	601	ARG	2.6
1	A	616	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	36	PRO	2.6
1	B	609	TYR	2.6
1	D	253	LYS	2.6
1	D	615	ASP	2.5
1	D	227	PRO	2.5
1	D	250	HIS	2.5
1	B	615	ASP	2.5
1	F	253	LYS	2.5
1	E	656	THR	2.5
1	C	86	HIS	2.4
1	C	653	VAL	2.4
1	D	66	LEU	2.4
1	C	250	HIS	2.4
1	F	340	HIS	2.4
1	D	135	MET	2.4
1	C	617	GLU	2.4
1	A	183	GLY	2.3
1	B	612	GLY	2.3
1	B	132	LEU	2.3
1	F	656	THR	2.3
1	A	1	MET	2.3
1	D	4	VAL	2.3
1	C	96	ALA	2.3
1	B	36	PRO	2.3
1	D	200	ARG	2.3
1	D	69	GLU	2.3
1	C	184	ASN	2.3
1	D	505	ARG	2.3
1	E	614	GLN	2.3
1	B	99	GLY	2.3
1	D	612	GLY	2.3
1	F	578	GLY	2.3
1	E	512	ILE	2.2
1	B	613	TYR	2.2
1	B	616	VAL	2.2
1	F	304	LEU	2.2
1	D	611	LYS	2.2
1	E	253	LYS	2.2
1	E	186	LEU	2.2
1	D	176	THR	2.2
1	E	36	PRO	2.2
1	C	650	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	249	PRO	2.1
1	A	89	TYR	2.1
1	C	253	LYS	2.1
1	D	83	TYR	2.1
1	F	89	TYR	2.1
1	D	199	GLY	2.1
1	F	183	GLY	2.1
1	F	250	HIS	2.1
1	D	111	TYR	2.1
1	C	507	GLY	2.1
1	E	250	HIS	2.1
1	A	619	ARG	2.1
1	D	128	THR	2.1
1	D	211	HIS	2.1
1	B	150	ILE	2.1
1	A	94	GLN	2.0
1	C	618	HIS	2.0
1	C	71	ILE	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	DTT	A	701[A]	8/8	0.79	0.17	32,55,55,55	18
2	DTT	A	701[B]	8/8	0.79	0.17	55,55,55,55	18
2	DTT	D	701[A]	8/8	0.80	0.16	35,64,64,64	18
2	DTT	D	701[B]	8/8	0.80	0.16	46,64,64,64	18
3	ACT	F	701	4/4	0.84	0.16	20,20,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ACT	A	702	4/4	0.91	0.14	20,20,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.