Full wwPDB X-ray Structure Validation Report (i)

Nov 1, 2021 – 12:56 PM EDT

PDB ID	:	2A27
Title	:	Human DRP-1 kinase, W305S S308A D40 mutant, crystal form with 8 monomers in the asymmetric unit
Authors	:	Kursula, P.; Lehmann, F.; Shani, G.; Kimchi, A.; Wilmanns, M.
Deposited on	:	2005-06-22
Resolution	:	3.00 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 (i) symbol.

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

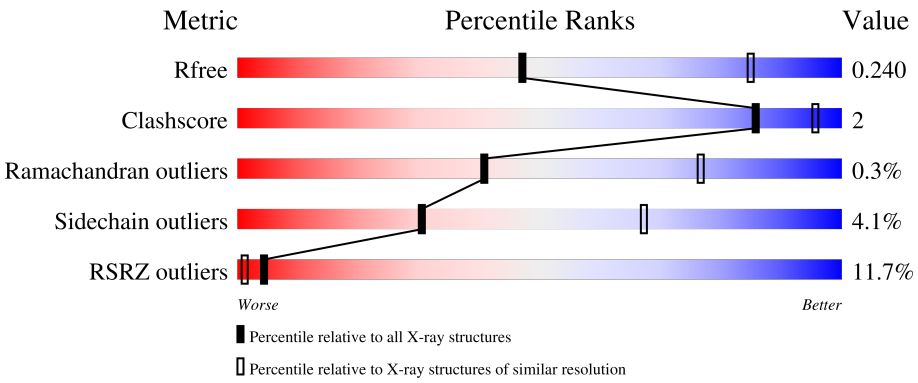
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	321	4%, 84%, 9%, • 5%
1	B	321	2%, 85%, 8%, • 6%
1	C	321	5%, 84%, 8%, • 6%
1	D	321	11%, 85%, 9%, • 5%
1	E	321	12%, 85%, 9%, • 6%

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Mol	Chain	Length	Quality of chain
1	F	321	20% 86% 8% 6%
1	G	321	17% 86% 7% • 6%
1	H	321	17% 85% 9% • 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DTT	A	1001	X	-	-	-
2	DTT	B	1002	X	-	-	-
2	DTT	C	1003	X	-	-	-
2	DTT	D	1004	X	-	-	-
2	DTT	E	1005	X	-	-	-
2	DTT	F	1007	X	-	-	-
2	DTT	G	1006	X	-	-	X
2	DTT	H	1008	X	-	-	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 20003 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 Death-associated protein kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	304	2478	1584	425	465	4	0	0	0
1	B	303	2467	1578	421	464	4	0	0	0
1	C	303	2467	1578	421	464	4	0	0	0
1	D	304	2478	1584	425	465	4	0	0	0
1	E	303	2467	1578	421	464	4	0	0	0
1	F	303	2467	1578	421	464	4	0	0	0
1	G	303	2467	1578	421	464	4	0	0	0
1	H	304	2472	1581	422	465	4	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	cloning artifact	UNP Q9UIK4
A	305	SER	TRP	engineered mutation	UNP Q9UIK4
A	308	ALA	SER	engineered mutation	UNP Q9UIK4
B	0	GLY	-	cloning artifact	UNP Q9UIK4
B	305	SER	TRP	engineered mutation	UNP Q9UIK4
B	308	ALA	SER	engineered mutation	UNP Q9UIK4
C	0	GLY	-	cloning artifact	UNP Q9UIK4
C	305	SER	TRP	engineered mutation	UNP Q9UIK4
C	308	ALA	SER	engineered mutation	UNP Q9UIK4
D	0	GLY	-	cloning artifact	UNP Q9UIK4
D	305	SER	TRP	engineered mutation	UNP Q9UIK4
D	308	ALA	SER	engineered mutation	UNP Q9UIK4
E	0	GLY	-	cloning artifact	UNP Q9UIK4

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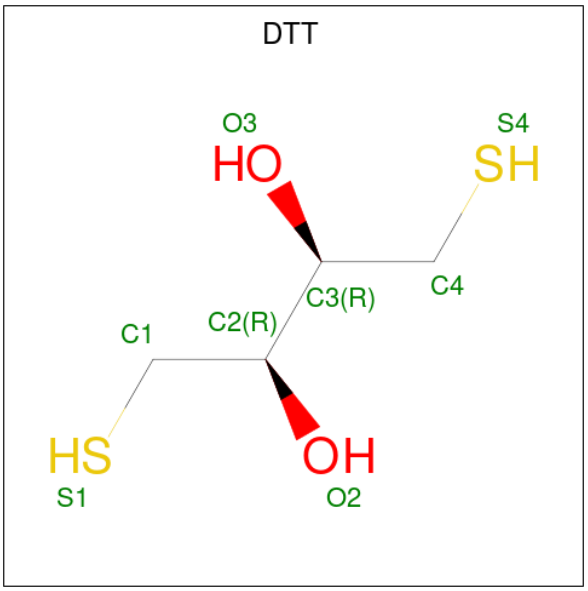
Chain	Residue	Modelled	Actual	Comment	Reference
E	305	SER	TRP	engineered mutation	UNP Q9UIK4
E	308	ALA	SER	engineered mutation	UNP Q9UIK4
F	0	GLY	-	cloning artifact	UNP Q9UIK4
F	305	SER	TRP	engineered mutation	UNP Q9UIK4
F	308	ALA	SER	engineered mutation	UNP Q9UIK4
G	0	GLY	-	cloning artifact	UNP Q9UIK4
G	305	SER	TRP	engineered mutation	UNP Q9UIK4
G	308	ALA	SER	engineered mutation	UNP Q9UIK4
H	0	GLY	-	cloning artifact	UNP Q9UIK4
H	305	SER	TRP	engineered mutation	UNP Q9UIK4
H	308	ALA	SER	engineered mutation	UNP Q9UIK4

- Molecule 2 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula: $C_4H_{10}O_2S_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
2	A	1	8	4	2	2	0	0
2	B	1	8	4	2	2	0	0
2	C	1	8	4	2	2	0	0
2	D	1	8	4	2	2	0	0
2	E	1	8	4	2	2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
2	F	1	8	4	2	2	0	0
			Total	C	O	S		
2	G	1	8	4	2	2	0	0
			Total	C	O	S		
2	H	1	8	4	2	2	0	0

- Molecule 3 is water.

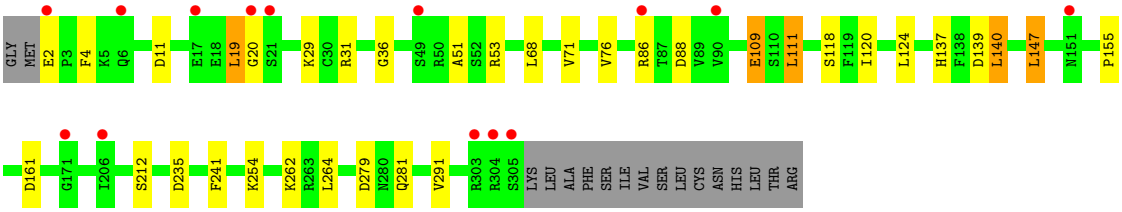
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	37	37	37	0	0
			Total	O		
3	B	55	55	55	0	0
			Total	O		
3	C	44	44	44	0	0
			Total	O		
3	D	17	17	17	0	0
			Total	O		
3	E	9	9	9	0	0
			Total	O		
3	F	3	3	3	0	0
			Total	O		
3	G	5	5	5	0	0
			Total	O		
3	H	6	6	6	0	0

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.

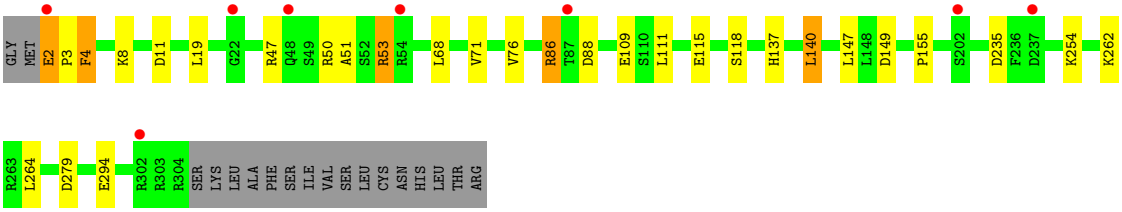
• Molecule 1: Death-associated protein kinase 2

Chain A:



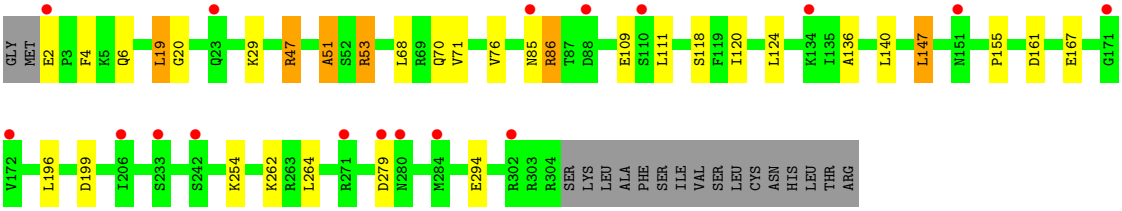
• Molecule 1: Death-associated protein kinase 2

Chain B:



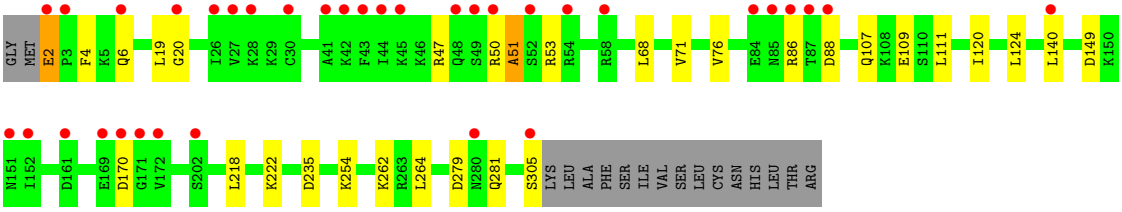
• Molecule 1: Death-associated protein kinase 2

Chain C:



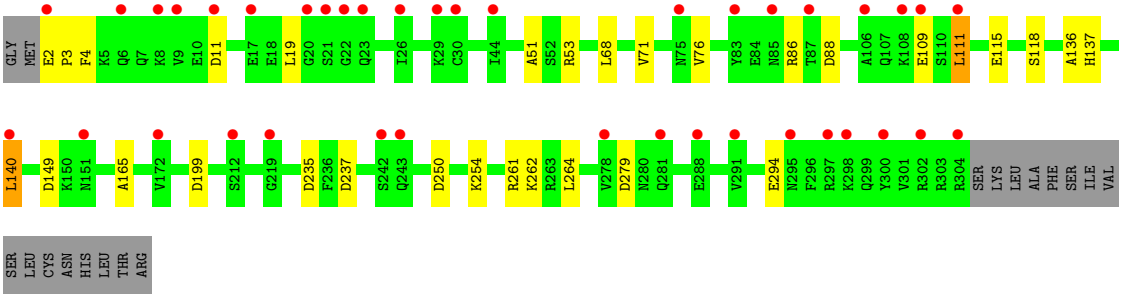
• Molecule 1: Death-associated protein kinase 2

Chain D:



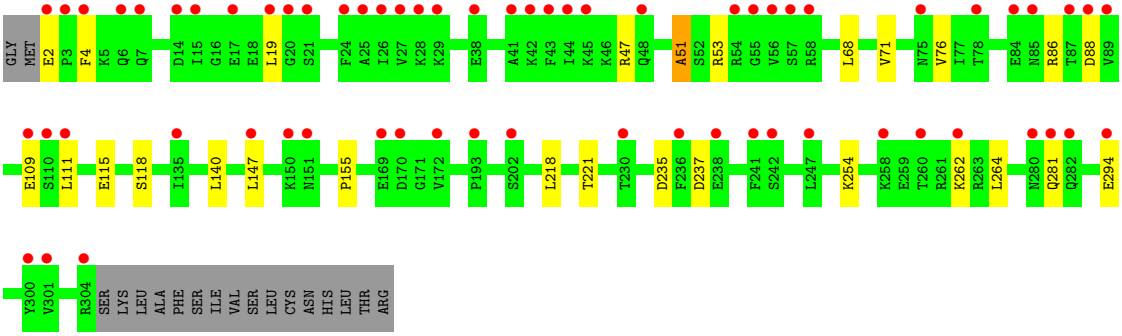
• Molecule 1: Death-associated protein kinase 2

Chain E:



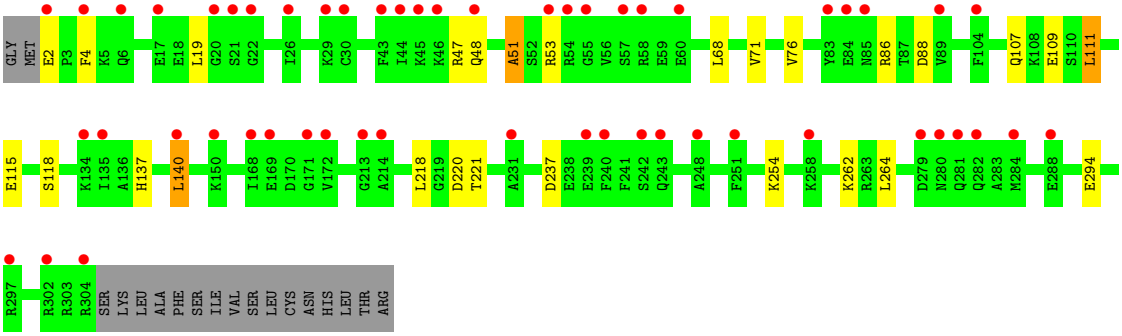
• Molecule 1: Death-associated protein kinase 2

Chain F:



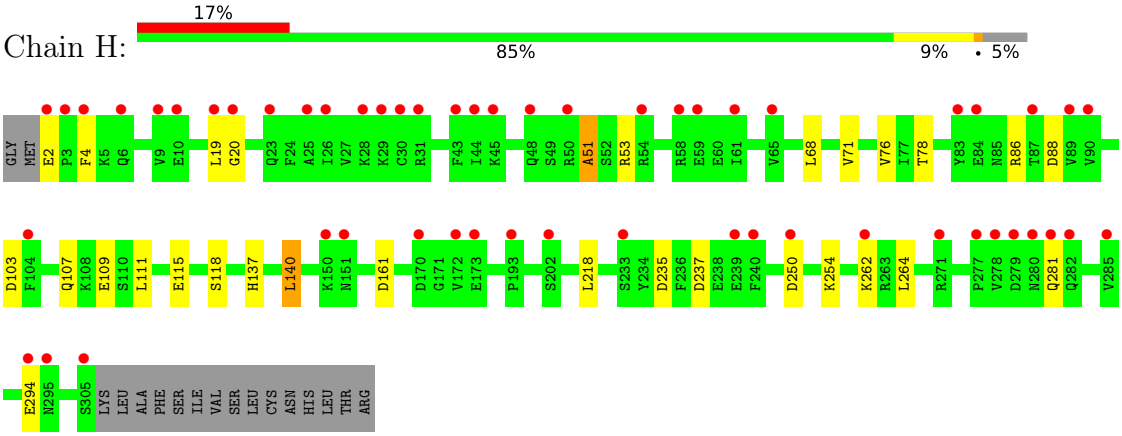
• Molecule 1: Death-associated protein kinase 2

Chain G:



• Molecule 1: Death-associated protein kinase 2

Chain H:


17%
85%
9%
5%
GLY MET E2 P3 F4 K5 Q6 V9 E10 L19 G20 Q23 F24 A25 I26 V27 K28 K29 C30 R31 F43 I44 K45 Q48 S49 R50 A51 S52 R53 R54 R58 E59 E60 I61 V65 L68 V71 V76 I77 T78 Y83 E84 N85 R86 T87 D88 V89 V90
D103 F104 Q107 K108 E109 S110 L111 E115 S118 H137 L140 K150 N151 D161 D170 G171 V172 E173 P193 S202 L218 S233 Y234 D235 F236 D237 E238 E239 F240 D250 K254 K262 R263 L264 R271 P277 V278 D279 N280 Q281 Q282 V285
E294 N295 S305 LYS LEU ALA PHE SER ILE VAL SER LEU CYS ASN HIS LEU THR ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	159.12Å 113.35Å 247.31Å 90.00° 95.09° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 33.46 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-3.00) 99.8 (33.46-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.16 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.2.0000	Depositor
R, R_{free}	0.217 , 0.238 0.218 , 0.240	Depositor DCC
R_{free} test set	4395 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	70.4	Xtriage
Anisotropy	0.581	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 111.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	20003	wwPDB-VP
Average B, all atoms (Å^2)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.58	0/2525	0.77	5/3405 (0.1%)
1	B	0.65	0/2514	0.79	5/3391 (0.1%)
1	C	0.49	0/2514	0.74	2/3391 (0.1%)
1	D	0.42	0/2525	0.71	5/3405 (0.1%)
1	E	0.38	0/2514	0.70	10/3391 (0.3%)
1	F	0.35	0/2514	0.67	3/3391 (0.1%)
1	G	0.34	0/2514	0.69	2/3391 (0.1%)
1	H	0.34	0/2519	0.68	6/3398 (0.2%)
All	All	0.46	0/20139	0.72	38/27163 (0.1%)

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	2
1	B	0	2
1	C	0	2
1	D	0	2
1	E	0	2
1	F	0	2
1	G	0	2
1	H	0	2
All	All	0	16

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	279	ASP	CB-CG-OD2	7.67	125.21	118.30
1	A	235	ASP	CB-CG-OD2	6.34	124.00	118.30
1	B	235	ASP	CB-CG-OD2	6.32	123.98	118.30
1	B	88	ASP	CB-CG-OD2	5.88	123.59	118.30
1	D	279	ASP	CB-CG-OD2	5.85	123.57	118.30
1	H	250	ASP	CB-CG-OD2	5.82	123.54	118.30
1	C	199	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	139	ASP	CB-CG-OD2	5.56	123.30	118.30
1	E	279	ASP	CB-CG-OD2	5.54	123.28	118.30
1	D	149	ASP	CB-CG-OD2	5.49	123.24	118.30
1	B	149	ASP	CB-CG-OD2	5.48	123.23	118.30
1	B	3	PRO	N-CA-C	5.44	126.25	112.10
1	E	11	ASP	CB-CG-OD2	5.39	123.16	118.30
1	E	235	ASP	CB-CG-OD2	5.37	123.14	118.30
1	F	88	ASP	CB-CG-OD2	5.35	123.11	118.30
1	H	235	ASP	CB-CG-OD2	5.26	123.03	118.30
1	E	237	ASP	CB-CG-OD2	5.22	123.00	118.30
1	E	88	ASP	CB-CG-OD2	5.19	122.97	118.30
1	E	149	ASP	CB-CG-OD2	5.18	122.96	118.30
1	H	237	ASP	CB-CG-OD2	5.18	122.96	118.30
1	D	88	ASP	CB-CG-OD2	5.17	122.96	118.30
1	B	279	ASP	CB-CG-OD2	5.17	122.96	118.30
1	G	237	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	11	ASP	CB-CG-OD2	5.16	122.94	118.30
1	D	235	ASP	CB-CG-OD2	5.15	122.93	118.30
1	F	235	ASP	CB-CG-OD2	5.14	122.93	118.30
1	E	261	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	G	88	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	88	ASP	CB-CG-OD2	5.11	122.89	118.30
1	H	161	ASP	CB-CG-OD2	5.10	122.89	118.30
1	C	279	ASP	CB-CG-OD2	5.10	122.89	118.30
1	H	88	ASP	CB-CG-OD2	5.09	122.89	118.30
1	E	199	ASP	CB-CG-OD2	5.06	122.86	118.30
1	D	170	ASP	CB-CG-OD2	5.04	122.84	118.30
1	E	3	PRO	N-CA-C	5.02	125.15	112.10
1	H	103	ASP	CB-CG-OD2	5.02	122.81	118.30
1	E	250	ASP	CB-CG-OD2	5.01	122.81	118.30
1	F	237	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2	GLU	Peptide
1	A	51	ALA	Peptide
1	B	2	GLU	Peptide
1	B	51	ALA	Peptide
1	C	2	GLU	Peptide
1	C	51	ALA	Peptide
1	D	2	GLU	Peptide
1	D	51	ALA	Peptide
1	E	2	GLU	Peptide
1	E	51	ALA	Peptide
1	F	2	GLU	Peptide
1	F	51	ALA	Peptide
1	G	2	GLU	Peptide
1	G	51	ALA	Peptide
1	H	2	GLU	Peptide
1	H	51	ALA	Peptide

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	2478	0	2489	13	0
1	B	2467	0	2476	12	0
1	C	2467	0	2476	12	0
1	D	2478	0	2489	16	0
1	E	2467	0	2476	6	0
1	F	2467	0	2476	9	0
1	G	2467	0	2476	15	0
1	H	2472	0	2478	9	0
2	A	8	0	8	2	0
2	B	8	0	8	0	0
2	C	8	0	8	0	0
2	D	8	0	10	0	0
2	E	8	0	8	1	0
2	F	8	0	10	1	0
2	G	8	0	10	1	0
2	H	8	0	10	2	0
3	A	37	0	0	1	0
3	B	55	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	44	0	0	1	0
3	D	17	0	0	1	0
3	E	9	0	0	0	0
3	F	3	0	0	0	0
3	G	5	0	0	0	0
3	H	6	0	0	1	0
All	All	20003	0	19908	89	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 2.

All (89) 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)
2:A:1001:DTT:S1	2:A:1001:DTT:S4	2.30	1.29
2:E:1005:DTT:S1	2:E:1005:DTT:S4	2.33	1.25
2:H:1008:DTT:HS2	2:H:1008:DTT:HS1	1.21	0.86
2:H:1008:DTT:S1	2:H:1008:DTT:S4	2.83	0.76
1:D:51:ALA:HB3	1:G:218:LEU:HD21	1.72	0.72
1:F:71:VAL:HG11	1:F:76:VAL:HG11	1.74	0.69
2:F:1007:DTT:S1	2:F:1007:DTT:S4	2.73	0.67
3:B:1042:HOH:O	1:C:51:ALA:HB1	1.95	0.66
1:B:4:PHE:HD1	1:B:4:PHE:H	1.44	0.66
1:D:254:LYS:HB3	1:D:264:LEU:HD13	1.80	0.63
1:D:51:ALA:HB2	1:G:218:LEU:HD11	1.82	0.61
1:G:254:LYS:HB3	1:G:264:LEU:HD13	1.83	0.60
1:D:218:LEU:HD21	1:G:51:ALA:HB3	1.82	0.60
1:F:254:LYS:HB3	1:F:264:LEU:HD13	1.82	0.60
1:A:109:GLU:HB2	3:A:1012:HOH:O	2.01	0.59
1:B:254:LYS:HB3	1:B:264:LEU:HD13	1.85	0.58
1:C:85:ASN:HD22	1:C:86:ARG:HD2	1.71	0.56
1:F:218:LEU:HD21	1:H:51:ALA:HB3	1.88	0.56
1:E:71:VAL:HG11	1:E:76:VAL:HG11	1.88	0.55
1:E:254:LYS:HB3	1:E:264:LEU:HD13	1.87	0.55
1:H:254:LYS:HB3	1:H:264:LEU:HD13	1.88	0.54
1:D:222:LYS:HE2	3:D:1007:HOH:O	2.08	0.53
1:C:254:LYS:HB3	1:C:264:LEU:HD13	1.91	0.53
1:D:305:SER:HA	1:G:48:GLN:HG3	1.91	0.53
1:D:47:ARG:NH2	1:G:220:ASP:O	2.42	0.53
1:C:71:VAL:HG11	1:C:76:VAL:HG11	1.92	0.52
1:A:254:LYS:HB3	1:A:264:LEU:HD13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:ILE:O	1:D:124:LEU:HG	2.10	0.51
1:H:71:VAL:HG11	1:H:76:VAL:HG11	1.91	0.51
1:A:71:VAL:HG11	1:A:76:VAL:HG11	1.93	0.51
1:B:71:VAL:HG12	1:B:71:VAL:O	2.12	0.50
1:A:4:PHE:CD1	1:A:4:PHE:N	2.80	0.49
2:A:1001:DTT:S4	2:A:1001:DTT:C1	2.99	0.49
1:B:47:ARG:NH1	1:B:50:ARG:HA	2.27	0.49
1:H:78:THR:HG22	3:H:1010:HOH:O	2.13	0.48
1:G:4:PHE:N	1:G:4:PHE:CD1	2.81	0.47
1:B:111:LEU:HD22	1:B:115:GLU:HB2	1.97	0.47
1:F:51:ALA:HB3	1:H:218:LEU:HD21	1.96	0.47
1:D:218:LEU:CD2	1:G:51:ALA:HB3	2.45	0.47
1:B:71:VAL:HG11	1:B:76:VAL:HG11	1.97	0.46
1:B:8:LYS:HB2	1:B:11:ASP:OD2	2.16	0.46
1:A:147:LEU:HG	1:A:155:PRO:HB2	1.98	0.45
1:C:4:PHE:N	1:C:4:PHE:CD1	2.84	0.45
1:G:137:HIS:HB3	1:G:140:LEU:HD13	1.98	0.45
1:H:4:PHE:CD1	1:H:4:PHE:N	2.84	0.45
1:H:115:GLU:O	1:H:118:SER:HB2	2.17	0.45
1:D:47:ARG:NH1	1:D:50:ARG:HA	2.32	0.45
1:A:4:PHE:N	1:A:4:PHE:HD1	2.15	0.45
1:B:137:HIS:CG	1:B:140:LEU:HD13	2.52	0.44
1:C:19:LEU:CD1	1:C:29:LYS:HB2	2.47	0.44
1:F:4:PHE:CD1	1:F:4:PHE:N	2.85	0.43
1:D:51:ALA:HB2	1:G:218:LEU:CD1	2.47	0.43
1:F:115:GLU:O	1:F:118:SER:HB2	2.19	0.43
1:C:53:ARG:HA	3:C:1028:HOH:O	2.18	0.43
1:F:71:VAL:CG1	1:F:76:VAL:HG11	2.44	0.43
1:H:137:HIS:HB3	1:H:140:LEU:HD13	2.01	0.43
1:A:19:LEU:CD1	1:A:29:LYS:HB2	2.49	0.43
1:A:120:ILE:O	1:A:124:LEU:HG	2.19	0.43
1:F:47:ARG:HB3	1:F:47:ARG:HH11	1.84	0.43
1:C:147:LEU:HG	1:C:155:PRO:HB2	2.00	0.43
1:D:71:VAL:HG11	1:D:76:VAL:HG11	2.00	0.43
1:G:4:PHE:N	1:G:4:PHE:HD1	2.16	0.42
1:B:53:ARG:HD2	3:B:1028:HOH:O	2.20	0.42
1:G:71:VAL:HG11	1:G:76:VAL:HG11	2.00	0.42
1:C:136:ALA:HB2	1:C:196:LEU:HD23	2.01	0.42
1:E:4:PHE:CD1	1:E:4:PHE:N	2.88	0.42
1:G:111:LEU:HD22	1:G:115:GLU:HB2	2.02	0.42
1:A:71:VAL:O	1:A:71:VAL:HG12	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:HIS:HB3	1:B:140:LEU:HD13	2.02	0.41
1:D:4:PHE:CD1	1:D:4:PHE:N	2.85	0.41
1:A:212:SER:HB3	1:A:241:PHE:CZ	2.55	0.41
1:D:71:VAL:HG12	1:D:71:VAL:O	2.18	0.41
1:A:137:HIS:HB3	1:A:140:LEU:HD13	2.01	0.41
1:B:147:LEU:HG	1:B:155:PRO:HB2	2.02	0.41
1:H:4:PHE:N	1:H:4:PHE:HD1	2.18	0.41
1:A:111:LEU:HD12	1:A:291:VAL:HG21	2.03	0.41
1:C:47:ARG:HH11	1:C:47:ARG:HB3	1.84	0.41
2:G:1006:DTT:S4	2:G:1006:DTT:S1	3.15	0.41
1:F:147:LEU:HG	1:F:155:PRO:HB2	2.03	0.41
1:A:31:ARG:NH1	1:A:36:GLY:O	2.53	0.41
1:E:136:ALA:O	1:E:165:ALA:HA	2.21	0.41
1:G:47:ARG:HH11	1:G:47:ARG:HB3	1.86	0.41
1:E:111:LEU:HD22	1:E:115:GLU:HB2	2.03	0.40
1:E:137:HIS:HB3	1:E:140:LEU:HD13	2.02	0.40
1:C:120:ILE:O	1:C:124:LEU:HG	2.21	0.40
1:D:2:GLU:OE2	1:D:2:GLU:HA	2.21	0.40
1:D:218:LEU:CD1	1:G:51:ALA:HB2	2.51	0.40
1:B:86:ARG:HD2	3:B:1013:HOH:O	2.22	0.40
1:C:70:GLN:NE2	1:C:167:GLU:OE1	2.52	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	302/321 (94%)	287 (95%)	13 (4%)	2 (1%)	22 60
1	B	301/321 (94%)	287 (95%)	13 (4%)	1 (0%)	41 76
1	C	301/321 (94%)	287 (95%)	12 (4%)	2 (1%)	22 60
1	D	302/321 (94%)	288 (95%)	13 (4%)	1 (0%)	41 76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	301/321 (94%)	289 (96%)	12 (4%)	0	100	100
1	F	301/321 (94%)	291 (97%)	10 (3%)	0	100	100
1	G	301/321 (94%)	293 (97%)	8 (3%)	0	100	100
1	H	302/321 (94%)	290 (96%)	11 (4%)	1 (0%)	41	76
All	All	2411/2568 (94%)	2312 (96%)	92 (4%)	7 (0%)	41	76

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	4	PHE
1	A	161	ASP
1	C	161	ASP
1	A	20	GLY
1	C	20	GLY
1	H	20	GLY
1	D	20	GLY

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	272/288 (94%)	261 (96%)	11 (4%)	31	68
1	B	271/288 (94%)	261 (96%)	10 (4%)	34	70
1	C	271/288 (94%)	258 (95%)	13 (5%)	25	62
1	D	272/288 (94%)	261 (96%)	11 (4%)	31	68
1	E	271/288 (94%)	261 (96%)	10 (4%)	34	70
1	F	271/288 (94%)	260 (96%)	11 (4%)	30	67
1	G	271/288 (94%)	259 (96%)	12 (4%)	28	65
1	H	271/288 (94%)	260 (96%)	11 (4%)	30	67
All	All	2170/2304 (94%)	2081 (96%)	89 (4%)	30	67

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	53	ARG
1	A	68	LEU
1	A	86	ARG
1	A	109	GLU
1	A	111	LEU
1	A	118	SER
1	A	140	LEU
1	A	147	LEU
1	A	262	LYS
1	A	281	GLN
1	B	2	GLU
1	B	19	LEU
1	B	53	ARG
1	B	68	LEU
1	B	86	ARG
1	B	109	GLU
1	B	118	SER
1	B	140	LEU
1	B	262	LYS
1	B	294	GLU
1	C	6	GLN
1	C	19	LEU
1	C	47	ARG
1	C	53	ARG
1	C	68	LEU
1	C	86	ARG
1	C	109	GLU
1	C	111	LEU
1	C	118	SER
1	C	140	LEU
1	C	147	LEU
1	C	262	LYS
1	C	294	GLU
1	D	6	GLN
1	D	19	LEU
1	D	53	ARG
1	D	68	LEU
1	D	86	ARG
1	D	107	GLN
1	D	109	GLU
1	D	111	LEU
1	D	140	LEU

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Mol	Chain	Res	Type
1	D	262	LYS
1	D	281	GLN
1	E	19	LEU
1	E	53	ARG
1	E	68	LEU
1	E	86	ARG
1	E	109	GLU
1	E	111	LEU
1	E	118	SER
1	E	140	LEU
1	E	262	LYS
1	E	294	GLU
1	F	19	LEU
1	F	53	ARG
1	F	68	LEU
1	F	86	ARG
1	F	109	GLU
1	F	111	LEU
1	F	140	LEU
1	F	221	THR
1	F	262	LYS
1	F	281	GLN
1	F	294	GLU
1	G	19	LEU
1	G	53	ARG
1	G	68	LEU
1	G	86	ARG
1	G	107	GLN
1	G	109	GLU
1	G	111	LEU
1	G	118	SER
1	G	140	LEU
1	G	221	THR
1	G	262	LYS
1	G	294	GLU
1	H	19	LEU
1	H	53	ARG
1	H	68	LEU
1	H	86	ARG
1	H	107	GLN
1	H	109	GLU
1	H	111	LEU

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Mol	Chain	Res	Type
1	H	140	LEU
1	H	262	LYS
1	H	281	GLN
1	H	294	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	85	ASN
1	A	144	ASN
1	A	223	GLN
1	A	267	GLN
1	B	23	GLN
1	B	144	ASN
1	B	223	GLN
1	B	267	GLN
1	B	281	GLN
1	C	6	GLN
1	C	23	GLN
1	C	85	ASN
1	C	144	ASN
1	C	223	GLN
1	D	23	GLN
1	D	70	GLN
1	D	144	ASN
1	D	223	GLN
1	E	6	GLN
1	E	23	GLN
1	E	70	GLN
1	E	85	ASN
1	E	144	ASN
1	E	223	GLN
1	E	267	GLN
1	F	23	GLN
1	F	85	ASN
1	F	144	ASN
1	F	223	GLN
1	G	6	GLN
1	G	23	GLN
1	G	70	GLN
1	G	85	ASN

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Mol	Chain	Res	Type
1	G	144	ASN
1	G	223	GLN
1	H	6	GLN
1	H	23	GLN
1	H	144	ASN
1	H	223	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	E	1005	-	7,7,7	0.53	0	4,8,8	1.15	0
2	DTT	D	1004	-	7,7,7	0.74	0	4,8,8	0.88	0
2	DTT	A	1001	-	7,7,7	0.57	0	4,8,8	0.82	0
2	DTT	G	1006	-	7,7,7	0.57	0	4,8,8	0.53	0
2	DTT	C	1003	-	7,7,7	0.59	0	4,8,8	0.77	0
2	DTT	H	1008	-	7,7,7	0.57	0	4,8,8	0.49	0
2	DTT	B	1002	-	7,7,7	0.67	0	4,8,8	0.68	0
2	DTT	F	1007	-	7,7,7	0.60	0	4,8,8	0.51	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	E	1005	-	1/1/2/2	5/8/8/8	-
2	DTT	D	1004	-	1/1/2/2	6/8/8/8	-
2	DTT	A	1001	-	1/1/2/2	3/8/8/8	-
2	DTT	G	1006	-	1/1/2/2	3/8/8/8	-
2	DTT	C	1003	-	1/1/2/2	4/8/8/8	-
2	DTT	H	1008	-	1/1/2/2	3/8/8/8	-
2	DTT	B	1002	-	1/1/2/2	4/8/8/8	-
2	DTT	F	1007	-	1/1/2/2	4/8/8/8	-

There are no bond length outliers.

There are no bond angle outliers.

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1001	DTT	C3
2	B	1002	DTT	C3
2	C	1003	DTT	C3
2	D	1004	DTT	C3
2	E	1005	DTT	C3
2	F	1007	DTT	C3
2	G	1006	DTT	C3
2	H	1008	DTT	C3

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	DTT	C1-C2-C3-C4
2	B	1002	DTT	C1-C2-C3-O3
2	B	1002	DTT	C1-C2-C3-C4
2	B	1002	DTT	O2-C2-C3-O3
2	B	1002	DTT	O2-C2-C3-C4
2	C	1003	DTT	S1-C1-C2-C3
2	C	1003	DTT	C1-C2-C3-C4
2	D	1004	DTT	C1-C2-C3-O3
2	D	1004	DTT	C1-C2-C3-C4
2	D	1004	DTT	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	D	1004	DTT	O2-C2-C3-C4
2	D	1004	DTT	C2-C3-C4-S4
2	D	1004	DTT	O3-C3-C4-S4
2	E	1005	DTT	C1-C2-C3-C4
2	F	1007	DTT	S1-C1-C2-C3
2	F	1007	DTT	C2-C3-C4-S4
2	F	1007	DTT	O3-C3-C4-S4
2	G	1006	DTT	S1-C1-C2-C3
2	G	1006	DTT	C2-C3-C4-S4
2	G	1006	DTT	O3-C3-C4-S4
2	H	1008	DTT	S1-C1-C2-C3
2	H	1008	DTT	C2-C3-C4-S4
2	H	1008	DTT	O3-C3-C4-S4
2	A	1001	DTT	C1-C2-C3-O3
2	E	1005	DTT	C1-C2-C3-O3
2	C	1003	DTT	O3-C3-C4-S4
2	E	1005	DTT	O3-C3-C4-S4
2	C	1003	DTT	C1-C2-C3-O3
2	E	1005	DTT	S1-C1-C2-C3
2	E	1005	DTT	C2-C3-C4-S4
2	A	1001	DTT	O2-C2-C3-O3
2	F	1007	DTT	C1-C2-C3-C4

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1005	DTT	1	0
2	A	1001	DTT	2	0
2	G	1006	DTT	1	0
2	H	1008	DTT	2	0
2	F	1007	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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	304/321 (94%)	0.66	14 (4%)	32	12	94, 99, 104, 121	0
1	B	303/321 (94%)	0.72	8 (2%)	56	27	94, 99, 104, 113	0
1	C	303/321 (94%)	0.72	17 (5%)	24	8	94, 99, 103, 111	0
1	D	304/321 (94%)	0.86	35 (11%)	4	1	95, 99, 103, 112	0
1	E	303/321 (94%)	0.92	39 (12%)	3	1	94, 99, 103, 109	0
1	F	303/321 (94%)	1.23	64 (21%)	1	0	96, 99, 103, 106	0
1	G	303/321 (94%)	1.04	53 (17%)	1	0	95, 99, 103, 106	0
1	H	304/321 (94%)	1.06	54 (17%)	1	0	95, 99, 103, 111	0
All	All	2427/2568 (94%)	0.90	284 (11%)	4	1	94, 99, 103, 121	0

All (284) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	48	GLN	8.2
1	H	25	ALA	7.1
1	D	48	GLN	6.9
1	F	21	SER	6.7
1	F	26	ILE	6.4
1	F	4	PHE	6.0
1	G	55	GLY	5.9
1	A	2	GLU	5.9
1	H	279	ASP	5.8
1	E	295	ASN	5.8
1	G	284	MET	5.4
1	G	213	GLY	5.2
1	E	2	GLU	5.2
1	H	281	GLN	5.1
1	G	280	ASN	5.0
1	H	45	LYS	4.9

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Mol	Chain	Res	Type	RSRZ
1	F	280	ASN	4.8
1	H	89	VAL	4.7
1	G	84	GLU	4.7
1	G	172	VAL	4.7
1	D	151	ASN	4.7
1	D	84	GLU	4.6
1	E	242	SER	4.6
1	F	304	ARG	4.6
1	D	20	GLY	4.5
1	H	172	VAL	4.5
1	E	26	ILE	4.4
1	G	26	ILE	4.4
1	H	83	TYR	4.3
1	C	2	GLU	4.2
1	E	83	TYR	4.2
1	F	150	LYS	4.2
1	H	4	PHE	4.2
1	F	44	ILE	4.1
1	D	52	SER	4.1
1	F	27	VAL	4.1
1	H	2	GLU	4.0
1	F	236	PHE	4.0
1	G	30	CYS	4.0
1	F	300	TYR	4.0
1	F	58	ARG	4.0
1	H	44	ILE	4.0
1	E	29	LYS	4.0
1	F	85	ASN	4.0
1	F	43	PHE	3.9
1	D	6	GLN	3.9
1	F	260	THR	3.9
1	F	89	VAL	3.8
1	F	170	ASP	3.8
1	E	20	GLY	3.8
1	D	171	GLY	3.8
1	C	284	MET	3.7
1	C	302	ARG	3.7
1	H	150	LYS	3.7
1	G	48	GLN	3.7
1	E	172	VAL	3.7
1	F	151	ASN	3.7
1	H	19	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	F	258	LYS	3.6
1	D	26	ILE	3.6
1	C	279	ASP	3.6
1	E	302	ARG	3.6
1	G	89	VAL	3.6
1	F	262	LYS	3.5
1	G	29	LYS	3.5
1	G	150	LYS	3.5
1	H	90	VAL	3.5
1	G	2	GLU	3.5
1	G	21	SER	3.5
1	F	301	VAL	3.4
1	H	10	GLU	3.4
1	H	151	ASN	3.4
1	F	45	LYS	3.4
1	H	20	GLY	3.4
1	H	193	PRO	3.4
1	D	2	GLU	3.4
1	H	30	CYS	3.4
1	H	239	GLU	3.4
1	F	54	ARG	3.4
1	C	134	LYS	3.4
1	D	140	LEU	3.3
1	G	243	GLN	3.3
1	F	111	LEU	3.3
1	H	29	LYS	3.3
1	F	172	VAL	3.3
1	F	110	SER	3.3
1	F	28	LYS	3.3
1	F	281	GLN	3.3
1	E	111	LEU	3.2
1	F	14	ASP	3.2
1	F	3	PRO	3.2
1	H	280	ASN	3.2
1	H	233	SER	3.2
1	E	17	GLU	3.2
1	F	2	GLU	3.2
1	H	84	GLU	3.2
1	G	171	GLY	3.1
1	D	58	ARG	3.1
1	H	50	ARG	3.1
1	G	304	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	11	ASP	3.1
1	F	241	PHE	3.1
1	E	106	ALA	3.1
1	B	302	ARG	3.1
1	A	305	SER	3.1
1	E	291	VAL	3.0
1	H	65	VAL	3.0
1	G	135	ILE	3.0
1	F	57	SER	3.0
1	D	43	PHE	3.0
1	H	202	SER	3.0
1	G	22	GLY	2.9
1	D	41	ALA	2.9
1	D	44	ILE	2.9
1	D	172	VAL	2.9
1	E	304	ARG	2.9
1	E	8	LYS	2.9
1	H	294	GLU	2.9
1	D	169	GLU	2.9
1	G	302	ARG	2.9
1	E	75	ASN	2.9
1	E	109	GLU	2.9
1	G	54	ARG	2.9
1	G	44	ILE	2.8
1	D	54	ARG	2.8
1	G	83	TYR	2.8
1	A	49	SER	2.8
1	F	7	GLN	2.8
1	H	6	GLN	2.8
1	H	278	VAL	2.8
1	F	19	LEU	2.8
1	E	140	LEU	2.8
1	G	214	ALA	2.8
1	F	20	GLY	2.8
1	G	134	LYS	2.8
1	G	248	ALA	2.8
1	D	28	LYS	2.8
1	H	9	VAL	2.8
1	F	84	GLU	2.7
1	H	59	GLU	2.7
1	G	168	ILE	2.7
1	H	262	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	22	GLY	2.7
1	C	171	GLY	2.7
1	F	6	GLN	2.7
1	H	170	ASP	2.7
1	G	251	PHE	2.7
1	H	26	ILE	2.7
1	D	88	ASP	2.7
1	F	247	LEU	2.7
1	B	2	GLU	2.7
1	F	202	SER	2.7
1	H	43	PHE	2.7
1	B	87	THR	2.6
1	E	6	GLN	2.6
1	D	45	LYS	2.6
1	A	86	ARG	2.6
1	G	4	PHE	2.6
1	D	87	THR	2.6
1	H	61	ILE	2.6
1	F	87	THR	2.6
1	G	20	GLY	2.6
1	D	50	ARG	2.6
1	C	242	SER	2.5
1	G	140	LEU	2.5
1	F	42	LYS	2.5
1	G	258	LYS	2.5
1	F	75	ASN	2.5
1	F	109	GLU	2.5
1	H	250	ASP	2.5
1	E	9	VAL	2.5
1	D	280	ASN	2.5
1	F	38	GLU	2.5
1	D	3	PRO	2.5
1	E	21	SER	2.5
1	C	280	ASN	2.5
1	B	237	ASP	2.5
1	E	243	GLN	2.5
1	A	21	SER	2.5
1	G	60	GLU	2.5
1	A	171	GLY	2.5
1	H	240	PHE	2.5
1	H	282	GLN	2.5
1	F	169	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	27	VAL	2.4
1	E	151	ASN	2.4
1	E	278	VAL	2.4
1	B	54	ARG	2.4
1	F	193	PRO	2.4
1	D	152	ILE	2.4
1	E	85	ASN	2.4
1	G	85	ASN	2.4
1	G	239	GLU	2.4
1	B	22	GLY	2.4
1	C	110	SER	2.4
1	F	135	ILE	2.4
1	F	282	GLN	2.4
1	D	30	CYS	2.4
1	F	230	THR	2.4
1	G	279	ASP	2.4
1	F	238	GLU	2.4
1	G	288	GLU	2.4
1	C	206	ILE	2.4
1	H	48	GLN	2.3
1	E	212	SER	2.3
1	F	147	LEU	2.3
1	H	295	ASN	2.3
1	H	271	ARG	2.3
1	D	42	LYS	2.3
1	F	25	ALA	2.3
1	H	87	THR	2.3
1	C	23	GLN	2.3
1	F	56	VAL	2.3
1	A	6	GLN	2.3
1	G	242	SER	2.3
1	G	297	ARG	2.3
1	C	233	SER	2.3
1	H	58	ARG	2.3
1	E	288	GLU	2.3
1	E	281	GLN	2.3
1	G	46	LYS	2.3
1	F	294	GLU	2.3
1	D	202	SER	2.3
1	E	300	TYR	2.3
1	A	17	GLU	2.3
1	F	41	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	57	SER	2.2
1	H	3	PRO	2.2
1	A	304	ARG	2.2
1	E	87	THR	2.2
1	G	17	GLU	2.2
1	F	15	ILE	2.2
1	G	281	GLN	2.2
1	F	24	PHE	2.2
1	F	242	SER	2.2
1	H	104	PHE	2.2
1	C	172	VAL	2.2
1	F	88	ASP	2.2
1	H	277	PRO	2.2
1	E	108	LYS	2.2
1	H	23	GLN	2.2
1	D	49	SER	2.2
1	A	90	VAL	2.2
1	G	104	PHE	2.2
1	D	86	ARG	2.2
1	C	88	ASP	2.1
1	C	85	ASN	2.1
1	E	297	ARG	2.1
1	D	170	ASP	2.1
1	G	240	PHE	2.1
1	F	29	LYS	2.1
1	G	282	GLN	2.1
1	H	305	SER	2.1
1	F	78	THR	2.1
1	H	285	VAL	2.1
1	D	305	SER	2.1
1	E	44	ILE	2.1
1	H	173	GLU	2.1
1	A	206	ILE	2.1
1	D	85	ASN	2.1
1	A	20	GLY	2.1
1	B	48	GLN	2.1
1	E	219	GLY	2.1
1	B	202	SER	2.1
1	G	43	PHE	2.1
1	G	6	GLN	2.1
1	G	58	ARG	2.1
1	H	31	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	23	GLN	2.1
1	G	45	LYS	2.1
1	G	231	ALA	2.1
1	C	271	ARG	2.1
1	G	169	GLU	2.0
1	H	28	LYS	2.0
1	D	161	ASP	2.0
1	F	17	GLU	2.0
1	C	151	ASN	2.0
1	A	303	ARG	2.0
1	H	54	ARG	2.0
1	A	151	ASN	2.0
1	G	53	ARG	2.0
1	F	55	GLY	2.0
1	E	298	LYS	2.0
1	E	30	CYS	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)

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	G	1006	8/8	0.70	0.45	134,136,137,139	0
2	DTT	H	1008	8/8	0.76	0.32	136,137,138,140	0
2	DTT	D	1004	8/8	0.81	0.21	114,117,118,119	0
2	DTT	A	1001	8/8	0.82	0.26	93,96,97,98	0
2	DTT	E	1005	8/8	0.86	0.36	102,103,104,104	0
2	DTT	F	1007	8/8	0.87	0.22	123,124,125,125	0
2	DTT	C	1003	8/8	0.93	0.17	74,79,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	DTT	B	1002	8/8	0.94	0.17	72,73,74,75	0

6.5 Other polymers (i)

There are no such residues in this entry.