Full wwPDB X-ray Structure Validation Report (i)

Nov 5, 2023 – 10:58 pm GMT

PDB ID	:	1W27
Title	:	Phenylalanine ammonia-lyase (PAL) from Petroselinum crispum
Authors	:	Ritter, H.; Schulz, G.E.
Deposited on	:	2004-06-29
Resolution	:	1.70 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 (i) 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 (1)) were used in the production of this report:

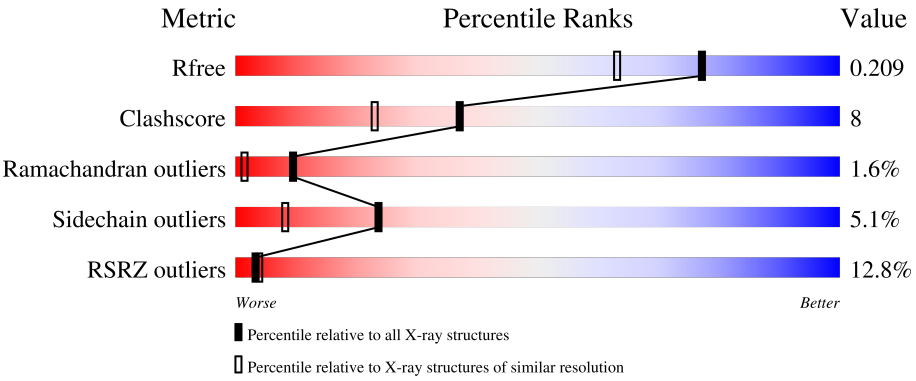
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.70 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}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 <=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	714	11% 83% 12%
1	B	714	13% 81% 13%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11663 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.

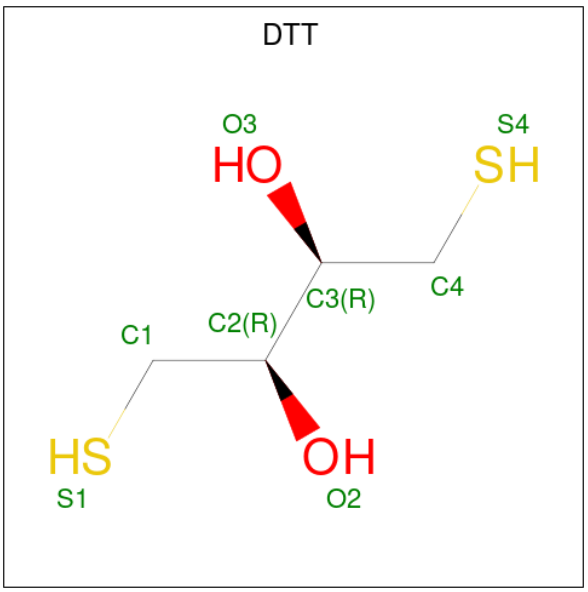
- Molecule 1 is a protein called PHENYLALANINE AMMONIA-LYASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	690	Total	C	N	O	S	0	0	0
			5288	3335	912	1014	27			
1	B	690	Total	C	N	O	S	0	0	0
			5288	3335	912	1014	27			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	203	MDO	ALA	modified residue	UNP P24481
A	203	MDO	SER	modified residue	UNP P24481
A	203	MDO	GLY	modified residue	UNP P24481
B	203	MDO	ALA	modified residue	UNP P24481
B	203	MDO	SER	modified residue	UNP P24481
B	203	MDO	GLY	modified residue	UNP P24481

- 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
2	A	1	Total	C	O	S	0	0
			8	4	2	2		
2	B	1	Total	C	O	S	0	0
			8	4	2	2		

- Molecule 3 is water.

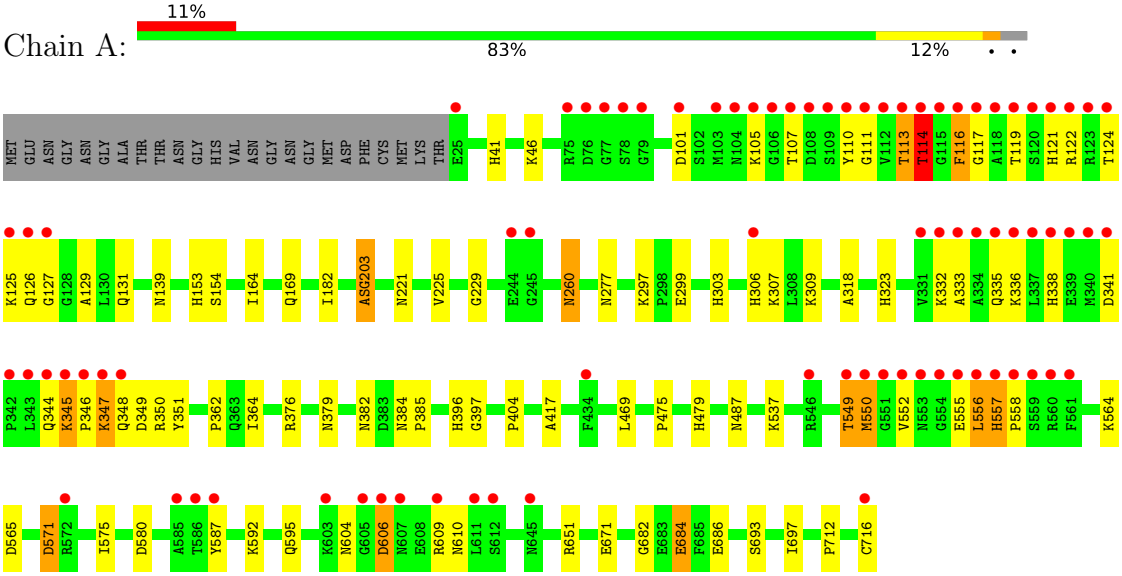
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	534	Total	O	0	0
			534	534		
3	B	537	Total	O	0	0
			537	537		

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.

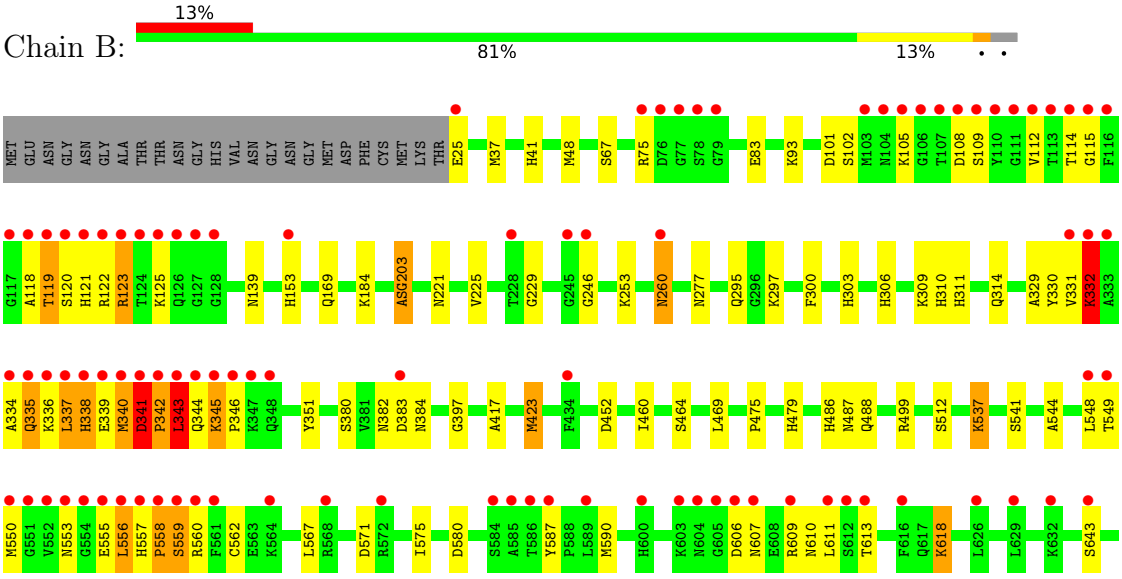
• Molecule 1: PHENYLALANINE AMMONIA-LYASE 1

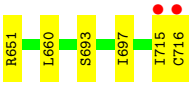
Chain A:



• Molecule 1: PHENYLALANINE AMMONIA-LYASE 1

Chain B:




R651
L660
S693
I697
I715
C716

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	119.96Å 160.81Å 141.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.70 19.98 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.3 (50.00-1.70) 98.4 (19.98-1.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.82 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.166 , 0.199 0.180 , 0.209	Depositor DCC
R_{free} test set	7349 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	18.9	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 55.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11663	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% 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

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

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	0.56	0/5369	0.74	5/7264 (0.1%)
1	B	0.57	1/5369 (0.0%)	0.73	7/7264 (0.1%)
All	All	0.56	1/10738 (0.0%)	0.74	12/14528 (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	B	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	423	MET	SD-CE	-10.63	1.18	1.77

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	565	ASP	CB-CG-OD2	6.38	124.04	118.30
1	B	580	ASP	CB-CG-OD2	5.76	123.48	118.30
1	A	101	ASP	CB-CG-OD2	5.71	123.44	118.30
1	B	341	ASP	CB-CG-OD2	5.70	123.43	118.30
1	B	101	ASP	CB-CG-OD2	5.56	123.31	118.30
1	B	108	ASP	CB-CG-OD2	5.41	123.16	118.30
1	A	580	ASP	CB-CG-OD2	5.30	123.07	118.30
1	B	499	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	B	452	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	606	ASP	CB-CG-OD2	5.10	122.89	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	571	ASP	CB-CG-OD2	5.09	122.88	118.30
1	B	606	ASP	CB-CG-OD2	5.08	122.87	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	246	GLY	Peptide
1	B	340	MET	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	5288	0	5309	79	0
1	B	5288	0	5309	99	2
2	A	8	0	9	1	0
2	B	8	0	9	1	0
3	A	534	0	0	18	1
3	B	537	0	0	28	1
All	All	11663	0	10636	166	3

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 8.

All (166) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:423:MET:SD	1:B:423:MET:CE	1.18	1.27
1:B:423:MET:SD	1:B:423:MET:HE2	1.76	1.14
1:B:423:MET:SD	1:B:423:MET:HE1	1.76	1.13
1:B:423:MET:SD	1:B:423:MET:HE3	1.76	1.10
1:A:306:HIS:HD2	1:A:318:ALA:CB	1.66	1.08
1:B:169:GLN:NE2	3:B:2166:HOH:O	1.84	1.06
1:B:153:HIS:CE1	1:B:225:VAL:HG11	1.93	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:423:MET:CE	1:B:423:MET:CG	2.38	1.01
1:B:41:HIS:HE1	1:B:277:ASN:HD22	1.07	1.00
1:A:306:HIS:CD2	1:A:318:ALA:CB	2.47	0.97
1:A:41:HIS:HE1	1:A:277:ASN:HD22	1.11	0.92
1:A:303:HIS:ND1	1:A:712:PRO:HG3	1.83	0.92
1:B:153:HIS:CD2	3:B:2150:HOH:O	2.24	0.91
1:A:306:HIS:CD2	1:A:318:ALA:HB2	2.06	0.90
1:B:332:LYS:HA	3:B:2301:HOH:O	1.76	0.84
1:B:169:GLN:HG3	3:B:2167:HOH:O	1.78	0.83
1:A:303:HIS:HD2	1:A:303:HIS:O	1.62	0.82
1:B:153:HIS:ND1	1:B:225:VAL:HG11	1.94	0.81
1:B:169:GLN:HG3	3:B:2168:HOH:O	1.79	0.81
1:A:693:SER:HB2	3:A:2510:HOH:O	1.80	0.80
1:A:303:HIS:CE1	1:A:712:PRO:HG3	2.17	0.79
1:A:113:THR:O	1:A:114:THR:OG1	2.00	0.78
1:A:154:SER:HB3	3:A:2061:HOH:O	1.84	0.76
1:B:41:HIS:HE1	1:B:277:ASN:ND2	1.83	0.76
1:B:41:HIS:CE1	1:B:277:ASN:HD22	1.99	0.75
1:B:380:SER:OG	1:B:382:ASN:ND2	2.19	0.75
1:A:303:HIS:O	1:A:303:HIS:CD2	2.39	0.75
1:B:537:LYS:HG3	1:B:567:LEU:HD22	1.66	0.75
1:A:309:LYS:HE3	1:B:382:ASN:ND2	2.02	0.74
1:A:303:HIS:ND1	1:A:712:PRO:CG	2.53	0.72
1:B:486:HIS:CD2	3:B:2396:HOH:O	2.42	0.72
1:B:697:ILE:HG22	3:B:2514:HOH:O	1.90	0.72
1:A:697:ILE:HG22	3:A:2511:HOH:O	1.90	0.70
1:B:423:MET:CE	1:B:423:MET:CB	2.70	0.69
1:A:41:HIS:HE1	1:A:277:ASN:ND2	1.89	0.69
1:B:423:MET:HE1	1:B:512:SER:HA	1.74	0.69
1:A:297:LYS:HG2	3:A:2266:HOH:O	1.93	0.68
1:A:41:HIS:CE1	1:A:277:ASN:HD22	2.03	0.68
1:A:303:HIS:CD2	1:A:307:LYS:HB2	2.28	0.68
1:B:75:ARG:NE	3:B:2064:HOH:O	2.26	0.68
1:B:693:SER:HB2	3:B:2513:HOH:O	1.93	0.68
1:B:423:MET:CE	1:B:423:MET:HB3	2.24	0.67
1:B:384:ASN:ND2	1:B:397:GLY:H	1.92	0.67
1:A:169:GLN:NE2	3:A:2162:HOH:O	2.22	0.65
1:A:107:THR:HG22	1:A:107:THR:O	1.97	0.64
1:B:486:HIS:CD2	1:B:486:HIS:N	2.66	0.64
1:A:344:GLN:NE2	1:A:347:LYS:O	2.31	0.63
1:A:475:PRO:HD3	1:B:475:PRO:HD3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:GLU:OE1	3:B:2076:HOH:O	2.15	0.63
1:A:139:ASN:HD22	1:A:221:ASN:HD21	1.48	0.61
1:B:342:PRO:HG3	3:B:2267:HOH:O	2.00	0.61
1:B:716:CYS:N	3:B:2536:HOH:O	2.34	0.60
1:B:487:ASN:HB2	3:B:2402:HOH:O	2.02	0.60
1:A:351:TYR:OH	1:B:203:MDO:HB21	2.02	0.60
1:B:544:ALA:HB1	1:B:548:LEU:HD12	1.83	0.59
1:A:203:MDO:HB21	1:B:351:TYR:OH	2.03	0.59
1:A:121:HIS:HB2	1:A:129:ALA:HB3	1.84	0.59
1:A:306:HIS:HD2	1:A:318:ALA:HB3	1.66	0.59
1:A:344:GLN:HE22	1:A:347:LYS:HG3	1.68	0.58
1:B:48:MET:HG3	1:B:67:SER:OG	2.04	0.58
1:A:404:PRO:HG2	1:B:311:HIS:CD2	2.39	0.58
1:A:303:HIS:ND1	1:A:712:PRO:CB	2.67	0.57
1:B:139:ASN:HD22	1:B:221:ASN:HD21	1.51	0.57
1:B:651:ARG:NH2	3:B:2474:HOH:O	2.38	0.57
1:B:479:HIS:HE1	3:B:2384:HOH:O	1.88	0.56
1:A:384:ASN:ND2	1:A:397:GLY:H	2.03	0.56
1:B:306:HIS:CD2	1:B:314:GLN:HE21	2.23	0.56
1:A:309:LYS:HE3	1:B:382:ASN:HD22	1.69	0.56
1:A:333:ALA:HB1	1:A:341:ASP:O	2.05	0.55
1:A:131:GLN:NE2	3:A:2120:HOH:O	2.27	0.55
1:B:341:ASP:HB2	1:B:342:PRO:CD	2.36	0.54
1:B:341:ASP:CB	1:B:342:PRO:CD	2.86	0.53
1:B:37:MET:HE1	3:B:2319:HOH:O	2.09	0.52
1:B:341:ASP:O	1:B:343:LEU:N	2.42	0.52
1:B:423:MET:HE2	1:B:423:MET:CB	2.39	0.52
1:B:558:PRO:O	1:B:559:SER:CB	2.57	0.52
1:B:153:HIS:HB3	3:B:2064:HOH:O	2.09	0.52
1:A:364:ILE:HD13	3:A:2284:HOH:O	2.10	0.51
1:B:297:LYS:HG2	1:B:343:LEU:HA	1.92	0.51
1:B:303:HIS:HB3	1:B:715:ILE:HG21	1.91	0.51
1:A:306:HIS:CD2	1:A:318:ALA:HB1	2.39	0.51
1:B:423:MET:HE2	1:B:423:MET:HB3	1.91	0.51
1:A:671:GLU:H	1:A:684:GLU:HG2	1.76	0.51
1:B:423:MET:HE3	1:B:423:MET:HB3	1.93	0.51
1:A:346:PRO:O	1:A:347:LYS:HG2	2.12	0.50
1:A:350:ARG:NE	3:A:2298:HOH:O	2.20	0.50
1:B:332:LYS:C	3:B:2300:HOH:O	2.49	0.50
1:A:299:GLU:OE2	1:A:345:LYS:NZ	2.40	0.50
1:A:323:HIS:HE1	3:A:2524:HOH:O	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:LYS:HE3	3:B:2093:HOH:O	2.12	0.49
1:B:306:HIS:HD2	1:B:314:GLN:HE21	1.59	0.49
1:B:329:ALA:O	1:B:332:LYS:HB2	2.12	0.49
1:B:460:ILE:HG22	3:B:2376:HOH:O	2.12	0.49
1:A:225:VAL:CG2	1:A:229:GLY:HA2	2.43	0.49
1:B:112:VAL:HG13	1:B:112:VAL:O	2.12	0.49
1:A:379:ASN:O	1:B:310:HIS:HE1	1.96	0.49
1:A:384:ASN:ND2	1:A:385:PRO:HA	2.27	0.49
1:A:479:HIS:HE1	3:A:2373:HOH:O	1.96	0.48
1:B:139:ASN:ND2	1:B:221:ASN:HD21	2.11	0.48
1:A:297:LYS:HZ2	1:A:349:ASP:HB2	1.78	0.48
1:B:303:HIS:HB3	1:B:715:ILE:CG2	2.43	0.48
1:A:153:HIS:CD2	3:A:2187:HOH:O	2.67	0.48
1:A:139:ASN:ND2	1:A:221:ASN:HD21	2.11	0.48
1:B:48:MET:CG	1:B:67:SER:OG	2.62	0.47
1:B:153:HIS:HE1	1:B:225:VAL:HG11	1.68	0.47
1:A:384:ASN:HD21	1:A:396:HIS:HA	1.80	0.47
1:A:417:ALA:HA	1:A:469:LEU:HG	1.98	0.46
1:A:404:PRO:CG	1:B:311:HIS:CD2	2.98	0.46
1:A:113:THR:C	1:A:114:THR:OG1	2.54	0.46
1:A:651:ARG:HH11	1:A:651:ARG:HG3	1.80	0.46
1:A:113:THR:HG22	1:A:114:THR:N	2.30	0.46
1:B:330:TYR:HA	1:B:651:ARG:HE	1.81	0.46
1:A:344:GLN:CG	3:A:2265:HOH:O	2.63	0.46
1:A:362:PRO:HG3	3:A:2283:HOH:O	2.15	0.46
1:B:331:VAL:HG23	3:B:2298:HOH:O	2.16	0.45
1:A:558:PRO:HD3	1:A:604:ASN:OD1	2.16	0.45
1:B:486:HIS:CD2	3:B:2399:HOH:O	2.68	0.45
1:B:118:ALA:O	1:B:119:THR:HG23	2.17	0.45
1:A:404:PRO:HG2	1:B:311:HIS:NE2	2.31	0.45
1:B:37:MET:CE	3:B:2319:HOH:O	2.63	0.45
1:B:550:MET:SD	1:B:618:LYS:NZ	2.81	0.45
1:A:303:HIS:HD2	1:A:307:LYS:HB2	1.79	0.44
1:A:306:HIS:HD2	1:A:318:ALA:HB1	1.67	0.44
1:A:348:GLN:NE2	3:A:2297:HOH:O	2.44	0.44
1:B:607:ASN:HD22	1:B:613:THR:HB	1.81	0.44
1:A:682:GLY:O	1:A:686:GLU:HG2	2.18	0.44
1:B:115:GLY:HA2	3:B:2116:HOH:O	2.17	0.44
1:B:153:HIS:CE1	1:B:225:VAL:CG1	2.84	0.44
1:B:300:PHE:O	1:B:306:HIS:HE1	2.01	0.44
1:B:384:ASN:HD21	1:B:397:GLY:H	1.62	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:HIS:HD2	3:A:2187:HOH:O	2.01	0.43
1:B:153:HIS:HD2	3:B:2150:HOH:O	1.81	0.43
1:A:303:HIS:CD2	1:A:303:HIS:C	2.91	0.43
1:A:107:THR:O	1:A:107:THR:CG2	2.67	0.43
1:B:41:HIS:HD2	3:B:2264:HOH:O	2.02	0.43
1:A:345:LYS:CB	1:A:346:PRO:CD	2.97	0.43
1:B:260:ASN:ND2	2:B:1717:DTT:S4	2.91	0.43
1:A:116:PHE:CD2	1:A:116:PHE:N	2.87	0.43
1:A:382:ASN:OD1	1:B:309:LYS:HE3	2.18	0.43
1:A:46:LYS:NZ	3:A:2029:HOH:O	2.28	0.42
1:A:549:THR:HA	1:A:556:LEU:CB	2.49	0.42
1:A:557:HIS:HA	1:A:558:PRO:HA	1.83	0.42
1:B:260:ASN:C	1:B:383:ASP:OD1	2.58	0.42
1:A:164:ILE:HD11	1:A:182:ILE:HG22	2.00	0.42
1:B:487:ASN:CB	3:B:2402:HOH:O	2.62	0.42
1:B:486:HIS:N	1:B:486:HIS:HD2	2.13	0.42
1:B:557:HIS:HA	1:B:558:PRO:HA	1.76	0.42
1:A:376:ARG:HB2	1:B:311:HIS:CE1	2.55	0.41
1:B:336:LYS:O	1:B:337:LEU:HG	2.20	0.41
1:B:225:VAL:CG2	1:B:229:GLY:HA2	2.49	0.41
1:A:260:ASN:ND2	2:A:1717:DTT:S4	2.93	0.41
1:A:487:ASN:HB2	3:A:2387:HOH:O	2.20	0.41
1:B:339:GLU:CB	1:B:571:ASP:HB3	2.49	0.41
1:B:464:SER:HB3	3:B:2376:HOH:O	2.20	0.41
1:B:555:GLU:O	1:B:556:LEU:C	2.59	0.41
1:A:41:HIS:HD2	3:A:2258:HOH:O	2.04	0.41
1:B:345:LYS:CB	1:B:346:PRO:HD3	2.51	0.41
1:B:417:ALA:HA	1:B:469:LEU:HG	2.02	0.41
1:B:334:ALA:O	1:B:340:MET:HG3	2.21	0.41
1:B:335:GLN:HG2	1:B:343:LEU:HB3	2.03	0.41
1:B:295:GLN:CD	1:B:341:ASP:HB3	2.41	0.40
1:B:341:ASP:HB2	1:B:342:PRO:HD2	2.02	0.40
1:B:541:SER:HB2	1:B:567:LEU:HD21	2.03	0.40
1:A:351:TYR:CE2	1:B:488:GLN:HG2	2.56	0.40
1:A:537:LYS:NZ	1:A:571:ASP:OD1	2.39	0.40
1:A:592:LYS:HA	1:A:595:GLN:HE21	1.86	0.40

All (3) 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)
1:B:486:HIS:ND1	1:B:486:HIS:ND1[3_555]	2.05	0.15
1:B:486:HIS:ND1	1:B:486:HIS:CE1[3_555]	2.11	0.09
3:A:2510:HOH:O	3:B:2131:HOH:O[3_555]	2.18	0.02

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	685/714 (96%)	646 (94%)	28 (4%)	11 (2%)	9 1
1	B	685/714 (96%)	643 (94%)	31 (4%)	11 (2%)	9 1
All	All	1370/1428 (96%)	1289 (94%)	59 (4%)	22 (2%)	9 1

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	THR
1	B	338	HIS
1	B	341	ASP
1	B	342	PRO
1	B	556	LEU
1	B	558	PRO
1	A	111	GLY
1	A	113	THR
1	A	119	THR
1	A	332	LYS
1	A	335	GLN
1	A	555	GLU
1	B	123	ARG
1	B	332	LYS
1	B	337	LEU
1	B	343	LEU
1	B	559	SER
1	A	124	THR

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Mol	Chain	Res	Type
1	A	127	GLY
1	B	335	GLN
1	A	550	MET
1	A	117	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	573/591 (97%)	548 (96%)	25 (4%)	28 11
1	B	573/591 (97%)	540 (94%)	33 (6%)	20 6
All	All	1146/1182 (97%)	1088 (95%)	58 (5%)	24 8

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	LYS
1	A	110	TYR
1	A	114	THR
1	A	116	PHE
1	A	122	ARG
1	A	125	LYS
1	A	126	GLN
1	A	260	ASN
1	A	336	LYS
1	A	338	HIS
1	A	345	LYS
1	A	347	LYS
1	A	549	THR
1	A	550	MET
1	A	552	VAL
1	A	556	LEU
1	A	557	HIS
1	A	564	LYS
1	A	575	ILE

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Mol	Chain	Res	Type
1	A	587	TYR
1	A	606	ASP
1	A	609	ARG
1	A	610	ASN
1	A	684	GLU
1	A	716	CYS
1	B	25	GLU
1	B	93	LYS
1	B	102	SER
1	B	105	LYS
1	B	109	SER
1	B	114	THR
1	B	119	THR
1	B	120	SER
1	B	121	HIS
1	B	122	ARG
1	B	123	ARG
1	B	125	LYS
1	B	253	LYS
1	B	260	ASN
1	B	332	LYS
1	B	338	HIS
1	B	343	LEU
1	B	344	GLN
1	B	345	LYS
1	B	537	LYS
1	B	549	THR
1	B	553	ASN
1	B	560	ARG
1	B	562	CYS
1	B	575	ILE
1	B	587	TYR
1	B	590	MET
1	B	609	ARG
1	B	610	ASN
1	B	611	LEU
1	B	618	LYS
1	B	643	SER
1	B	660	LEU

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	41	HIS
1	A	121	HIS
1	A	139	ASN
1	A	145	ASN
1	A	153	HIS
1	A	165	ASN
1	A	260	ASN
1	A	277	ASN
1	A	306	HIS
1	A	314	GLN
1	A	323	HIS
1	A	335	GLN
1	A	344	GLN
1	A	348	GLN
1	A	363	GLN
1	A	384	ASN
1	A	479	HIS
1	A	591	GLN
1	A	595	GLN
1	A	610	ASN
1	B	41	HIS
1	B	139	ASN
1	B	145	ASN
1	B	153	HIS
1	B	165	ASN
1	B	169	GLN
1	B	260	ASN
1	B	277	ASN
1	B	306	HIS
1	B	310	HIS
1	B	344	GLN
1	B	363	GLN
1	B	382	ASN
1	B	384	ASN
1	B	396	HIS
1	B	479	HIS
1	B	591	GLN
1	B	595	GLN
1	B	607	ASN
1	B	610	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	MDO	B	203	2,1	12,13,14	2.39	5 (41%)	15,18,20	3.67	7 (46%)
1	MDO	A	203	2,1	12,13,14	2.12	3 (25%)	15,18,20	3.84	6 (40%)

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
1	MDO	B	203	2,1	-	2/4/23/24	0/1/1/1
1	MDO	A	203	2,1	-	1/4/23/24	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	203	MDO	O2-C2	5.11	1.33	1.23
1	B	203	MDO	O2-C2	5.05	1.33	1.23
1	B	203	MDO	C2-N3	-3.92	1.30	1.39
1	A	203	MDO	C2-N3	-3.61	1.31	1.39
1	B	203	MDO	C1-N3	-2.71	1.32	1.37
1	B	203	MDO	CA2-N2	-2.63	1.34	1.39
1	A	203	MDO	C1-N3	-2.48	1.32	1.37
1	B	203	MDO	CA2-C2	-2.48	1.38	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	203	MDO	CA2-C2-N3	11.77	108.93	103.37
1	A	203	MDO	CA2-C2-N3	11.49	108.80	103.37
1	A	203	MDO	O2-C2-CA2	-5.86	127.67	130.96
1	A	203	MDO	C2-CA2-N2	-4.80	105.57	108.93
1	B	203	MDO	C2-CA2-N2	-4.00	106.13	108.93
1	B	203	MDO	O2-C2-CA2	-3.96	128.74	130.96
1	A	203	MDO	CB2-CA2-C2	3.90	129.89	122.76
1	B	203	MDO	CB2-CA2-C2	3.47	129.12	122.76
1	B	203	MDO	N3-C1-N2	-2.36	109.82	111.45
1	B	203	MDO	CA1-C1-N2	2.21	126.89	124.05
1	A	203	MDO	CA1-C1-N2	2.16	126.81	124.05
1	B	203	MDO	CA2-N2-C1	2.09	107.29	105.40
1	A	203	MDO	CA2-N2-C1	2.07	107.27	105.40

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	203	MDO	N2-C1-CA1-CB
1	B	203	MDO	N2-C1-CA1-CB
1	B	203	MDO	N3-C1-CA1-CB

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	203	MDO	1	0
1	A	203	MDO	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	1717	1	7,7,7	0.83	0	4,8,8	0.53	0
2	DTT	B	1717	1	7,7,7	0.69	0	4,8,8	1.26	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	A	1717	1	-	1/8/8/8	-
2	DTT	B	1717	1	-	0/8/8/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1717	DTT	S1-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1717	DTT	1	0
2	B	1717	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, 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	689/714 (96%)	0.88	81 (11%) 4 5	11, 20, 56, 63	0
1	B	689/714 (96%)	1.07	96 (13%) 2 3	11, 20, 57, 62	0
All	All	1378/1428 (96%)	0.97	177 (12%) 3 4	11, 20, 57, 63	0

All (177) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	343	LEU	20.7
1	A	112	VAL	18.6
1	B	118	ALA	18.3
1	B	337	LEU	17.8
1	A	343	LEU	17.1
1	B	110	TYR	17.1
1	B	107	THR	16.9
1	B	552	VAL	16.8
1	A	124	THR	16.8
1	A	337	LEU	16.6
1	B	115	GLY	16.3
1	B	119	THR	15.6
1	B	120	SER	15.1
1	A	110	TYR	14.9
1	B	124	THR	14.9
1	B	561	PHE	14.7
1	B	112	VAL	14.2
1	A	118	ALA	13.6
1	A	106	GLY	13.4
1	A	557	HIS	13.4
1	A	342	PRO	13.3
1	B	554	GLY	13.3
1	A	552	VAL	13.1
1	B	557	HIS	12.6

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Mol	Chain	Res	Type	RSRZ
1	B	553	ASN	12.4
1	A	115	GLY	12.4
1	A	551	GLY	12.2
1	B	106	GLY	12.2
1	A	111	GLY	12.1
1	B	556	LEU	12.1
1	A	107	THR	12.0
1	A	558	PRO	11.8
1	A	119	THR	11.7
1	B	550	MET	11.7
1	B	716	CYS	11.7
1	B	121	HIS	11.6
1	B	347	LYS	11.5
1	B	338	HIS	11.2
1	B	122	ARG	11.1
1	B	340	MET	11.1
1	B	125	LYS	10.8
1	A	550	MET	10.8
1	B	346	PRO	10.7
1	A	346	PRO	10.6
1	A	338	HIS	10.2
1	A	127	GLY	10.2
1	B	551	GLY	9.9
1	B	344	GLN	9.8
1	A	108	ASP	9.7
1	A	126	GLN	9.6
1	B	108	ASP	9.6
1	A	113	THR	9.4
1	A	121	HIS	9.4
1	B	123	ARG	9.3
1	A	345	LYS	9.3
1	A	339	GLU	9.2
1	A	340	MET	9.2
1	B	558	PRO	9.2
1	B	113	THR	9.1
1	A	120	SER	9.0
1	B	117	GLY	9.0
1	B	334	ALA	8.9
1	A	109	SER	8.8
1	B	126	GLN	8.8
1	B	342	PRO	8.7
1	B	345	LYS	8.6

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Mol	Chain	Res	Type	RSRZ
1	A	125	LYS	8.5
1	B	109	SER	8.5
1	B	341	ASP	8.4
1	A	554	GLY	8.4
1	A	123	ARG	8.4
1	A	116	PHE	8.3
1	B	114	THR	8.2
1	A	716	CYS	8.2
1	A	122	ARG	8.2
1	B	116	PHE	8.1
1	B	335	GLN	8.0
1	B	339	GLU	7.9
1	A	335	GLN	7.8
1	A	341	ASP	7.8
1	B	111	GLY	7.7
1	B	127	GLY	7.7
1	A	336	LYS	7.5
1	A	105	LYS	7.5
1	B	560	ARG	7.4
1	B	336	LYS	6.9
1	A	344	GLN	6.8
1	A	347	LYS	6.6
1	A	553	ASN	6.4
1	A	560	ARG	6.1
1	A	114	THR	6.0
1	B	105	LYS	5.9
1	B	332	LYS	5.8
1	B	331	VAL	5.8
1	A	555	GLU	5.8
1	B	348	GLN	5.8
1	B	549	THR	5.8
1	A	334	ALA	5.7
1	B	25	GLU	5.6
1	A	117	GLY	5.4
1	B	77	GLY	5.3
1	A	609	ARG	5.1
1	A	556	LEU	5.1
1	A	549	THR	5.0
1	B	104	ASN	4.9
1	B	715	ILE	4.8
1	B	555	GLU	4.7
1	B	609	ARG	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	333	ALA	4.4
1	A	606	ASP	4.3
1	B	585	ALA	4.3
1	B	78	SER	4.2
1	B	606	ASP	4.1
1	B	333	ALA	4.0
1	B	548	LEU	3.9
1	A	586	THR	3.9
1	A	645	ASN	3.9
1	B	586	THR	3.8
1	A	561	PHE	3.8
1	B	611	LEU	3.8
1	B	607	ASN	3.7
1	B	643	SER	3.7
1	B	603	LYS	3.7
1	A	559	SER	3.7
1	B	79	GLY	3.6
1	B	153	HIS	3.6
1	B	76	ASP	3.5
1	B	605	GLY	3.4
1	B	629	LEU	3.4
1	B	75	ARG	3.4
1	A	611	LEU	3.3
1	A	79	GLY	3.3
1	A	245	GLY	3.3
1	B	103	MET	3.3
1	A	76	ASP	3.2
1	A	605	GLY	3.2
1	B	587	TYR	3.2
1	A	25	GLU	3.2
1	A	77	GLY	3.2
1	A	434	PHE	3.1
1	A	104	ASN	3.0
1	B	616	PHE	3.0
1	A	103	MET	3.0
1	B	559	SER	3.0
1	B	612	SER	2.9
1	A	585	ALA	2.9
1	A	612	SER	2.8
1	A	603	LYS	2.8
1	A	546	ARG	2.7
1	A	348	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	246	GLY	2.7
1	A	332	LYS	2.7
1	B	604	ASN	2.7
1	B	589	LEU	2.6
1	A	78	SER	2.6
1	B	383	ASP	2.6
1	B	584	SER	2.5
1	B	626	LEU	2.5
1	B	228	THR	2.5
1	B	568	ARG	2.4
1	B	564	LYS	2.4
1	B	600	HIS	2.4
1	B	434	PHE	2.3
1	A	306	HIS	2.3
1	A	75	ARG	2.3
1	A	244	GLU	2.2
1	B	632	LYS	2.2
1	A	101	ASP	2.2
1	B	613	THR	2.2
1	B	572	ARG	2.1
1	B	245	GLY	2.1
1	A	572	ARG	2.1
1	A	587	TYR	2.1
1	B	128	GLY	2.1
1	A	607	ASN	2.1
1	B	260	ASN	2.1
1	A	331	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} 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
1	MDO	A	203	13/14	0.92	0.09	14,15,20,27	0
1	MDO	B	203	13/14	0.94	0.09	13,15,19,29	0

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, 95^{th} 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	B	1717	8/8	0.88	0.15	34,40,42,43	0
2	DTT	A	1717	8/8	0.93	0.14	30,35,37,40	0

6.5 Other polymers (i)

There are no such residues in this entry.