



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:09 AM UTC

PDB ID : 1W27 / pdb_00001w27
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 ⓘ 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

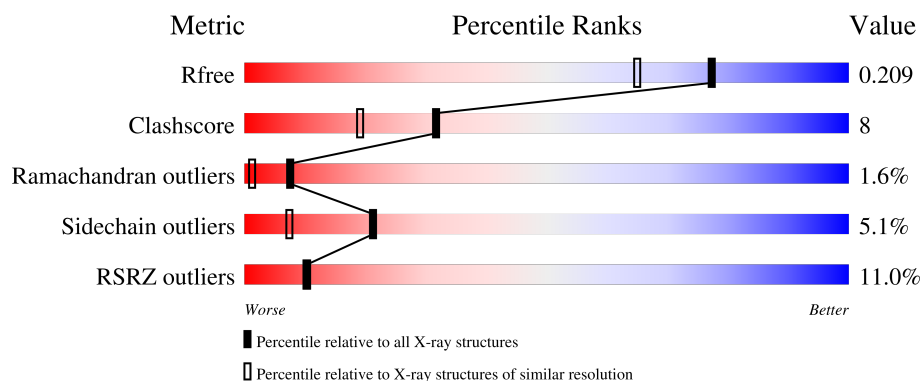
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (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 $\leq 5\%$. 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	714	9% 82% 13% • •
1	B	714	12% 82% 12% • •

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.

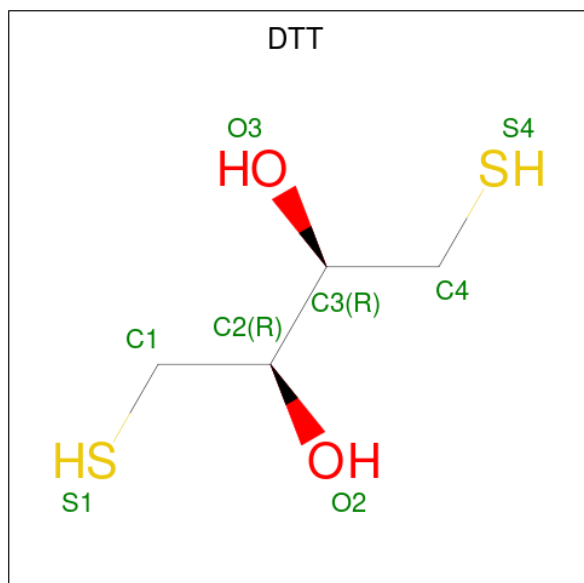
- Molecule 1 is a protein called PHENYLALANINE AMMONIA-LYASE 1.

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 (CCD ID: 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		

4 Data and refinement statistics

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 50.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.3 (50.00-1.70) 98.3 (50.00-1.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.39 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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.*

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: MDO, 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	0.75	5/5369 (0.1%)	0.85	0/7264
1	B	0.80	3/5369 (0.1%)	0.86	2/7264 (0.0%)
All	All	0.78	8/10738 (0.1%)	0.85	2/14528 (0.0%)

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 (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	423	MET	SD-CE	-24.49	1.18	1.79
1	B	37	MET	SD-CE	-7.46	1.60	1.79
1	A	271	MET	SD-CE	-7.14	1.61	1.79
1	A	318	ALA	CA-CB	-7.03	1.42	1.53
1	A	340	MET	CA-C	6.79	1.55	1.52
1	A	692	MET	SD-CE	-5.89	1.64	1.79
1	B	271	MET	SD-CE	-5.70	1.65	1.79
1	A	511	MET	SD-CE	-5.44	1.66	1.79

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	715	ILE	CB-CA-C	-5.67	105.09	110.70
1	B	263	ALA	N-CA-C	5.46	117.99	111.71

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

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	83	0
1	B	5288	0	5309	100	2
2	A	8	0	9	1	0
2	B	8	0	9	2	0
3	A	534	0	0	18	1
3	B	537	0	0	28	1
All	All	11663	0	10636	171	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 (171) 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:HE3	1.76	1.12
1:B:423:MET:SD	1:B:423:MET:HE2	1.76	1.11
1:A:306:HIS:HD2	1:A:318:ALA:CB	1.66	1.08
1:B:423:MET:SD	1:B:423:MET:HE1	1.76	1.06
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:37:MET:HE1	3:B:2319:HOH:O	1.80	0.81
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: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:46:LYS:NZ	3:A:2029:HOH:O	2.28	0.66
1:A:169:GLN:NE2	3:A:2162:HOH:O	2.22	0.65
1:B:423:MET:HE1	1:B:512:SER:HA	1.78	0.65
1:B:486:HIS:CD2	1:B:486:HIS:N	2.66	0.64
1:B:423:MET:HE2	1:B:423:MET:HB3	1.78	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
1:B:83:GLU:OE1	3:B:2076:HOH:O	2.15	0.63
1:B:423:MET:HE2	1:B:423:MET:CB	2.28	0.63
1:A:107:THR:HG22	1:A:107:THR:O	1.97	0.62
1:A:139:ASN:HD22	1:A:221:ASN:HD21	1.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:299:GLU:OE2	1:A:345:LYS:NZ	2.40	0.55
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:332:LYS:C	3:B:2300:HOH:O	2.49	0.54
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:341:ASP:O	1:B:343:LEU:N	2.42	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:A:113:THR:C	1:A:114:THR:OG1	2.54	0.51
1:A:671:GLU:H	1:A:684:GLU:HG2	1.76	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:A:323:HIS:HE1	3:A:2524:HOH:O	1.94	0.50
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:303:HIS:CD2	1:A:303:HIS:C	2.91	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:260:ASN:C	1:B:383:ASP:OD1	2.58	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: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:A:103:MET:HE2	1:A:122:ARG:HB3	1.98	0.45
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:B:295:GLN:CD	1:B:341:ASP:HB3	2.41	0.45
1:A:404:PRO:HG2	1:B:311:HIS:NE2	2.31	0.45
1:B:555:GLU:O	1:B:556:LEU:C	2.59	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:260:ASN:CG	2:B:1717:DTT:S4	3.00	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:TYR:C	1:B:332:LYS:N	2.75	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:B:103:MET:HE2	1:B:122:ARG:HD3	2.01	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: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:A:309:LYS:C	1:A:310:HIS:CD2	2.98	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: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:A:715:ILE:O	1:A:716:CYS:C	2.62	0.41
1:B:335:GLN:HG2	1:B:343:LEU:HB3	2.03	0.41
1:B:341:ASP:HB2	1:B:342:PRO:HD2	2.02	0.40
1:A:110:TYR:O	1:A:111:GLY:C	2.64	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:409:MET:HA	1:A:409:MET:HE2	2.02	0.40
1:A:592:LYS:HA	1:A:595:GLN:HE21	1.86	0.40
1:B:715:ILE:C	3:B:2536:HOH:O	2.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	7 1
1	B	685/714 (96%)	643 (94%)	31 (4%)	11 (2%)	7 1
All	All	1370/1428 (96%)	1289 (94%)	59 (4%)	22 (2%)	7 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 ⓘ

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%)	546 (95%)	27 (5%)	23	9
1	B	573/591 (97%)	541 (94%)	32 (6%)	19	6
All	All	1146/1182 (97%)	1087 (95%)	59 (5%)	21	7

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	GLU
1	A	37	MET
1	A	105	LYS
1	A	114	THR
1	A	116	PHE
1	A	122	ARG
1	A	125	LYS
1	A	126	GLN
1	A	275	GLU
1	A	336	LYS
1	A	338	HIS
1	A	345	LYS
1	A	347	LYS
1	A	546	ARG
1	A	549	THR
1	A	550	MET
1	A	552	VAL
1	A	556	LEU
1	A	564	LYS

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Mol	Chain	Res	Type
1	A	575	ILE
1	A	587	TYR
1	A	606	ASP
1	A	609	ARG
1	A	610	ASN
1	A	667	GLU
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	122	ARG
1	B	123	ARG
1	B	125	LYS
1	B	260	ASN
1	B	332	LYS
1	B	336	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	572	ARG
1	B	575	ILE
1	B	587	TYR
1	B	590	MET
1	B	611	LEU
1	B	617	GLN
1	B	618	LYS
1	B	627	LYS
1	B	660	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
1	A	126	GLN
1	A	139	ASN
1	A	145	ASN
1	A	153	HIS
1	A	169	GLN
1	A	306	HIS
1	A	310	HIS
1	A	323	HIS
1	A	335	GLN
1	A	344	GLN
1	A	348	GLN
1	A	384	ASN
1	A	479	HIS
1	A	591	GLN
1	A	595	GLN
1	A	600	HIS
1	A	610	ASN
1	B	41	HIS
1	B	139	ASN
1	B	145	ASN
1	B	153	HIS
1	B	251	GLN
1	B	306	HIS
1	B	310	HIS
1	B	344	GLN
1	B	382	ASN
1	B	384	ASN
1	B	396	HIS
1	B	479	HIS
1	B	487	ASN
1	B	591	GLN
1	B	607	ASN
1	B	610	ASN
1	B	645	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	1	11,13,14	2.58	5 (45%)	15,18,20	2.45	6 (40%)
1	MDO	A	203	1	11,13,14	2.28	3 (27%)	15,18,20	2.70	5 (33%)

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	1	-	2/4/23/24	0/1/1/1
1	MDO	A	203	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	5.31	1.33	1.23
1	B	203	MDO	O2-C2	5.24	1.33	1.23
1	B	203	MDO	C2-N3	-4.07	1.30	1.40
1	A	203	MDO	C2-N3	-3.76	1.31	1.40
1	B	203	MDO	C1-N3	-2.84	1.32	1.37
1	B	203	MDO	CA2-N2	-2.83	1.34	1.39
1	A	203	MDO	C1-N3	-2.60	1.32	1.37
1	B	203	MDO	CA2-C2	-2.50	1.38	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	203	MDO	CA2-C2-N3	6.47	108.93	103.50
1	A	203	MDO	CA2-C2-N3	6.32	108.80	103.50
1	A	203	MDO	O2-C2-CA2	-5.25	127.67	131.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	MDO	C2-CA2-N2	-4.72	105.57	108.95
1	B	203	MDO	C2-CA2-N2	-3.93	106.13	108.95
1	B	203	MDO	O2-C2-CA2	-3.58	128.74	131.02
1	B	203	MDO	CA1-C1-N2	2.28	126.89	124.04
1	A	203	MDO	CA1-C1-N2	2.22	126.81	124.04
1	B	203	MDO	CA2-N2-C1	2.12	107.29	105.39
1	B	203	MDO	N3-C1-N2	-2.11	109.82	111.48
1	A	203	MDO	CA2-N2-C1	2.09	107.27	105.39

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 oligosaccharides 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	B	1717	-	7,7,7	0.72	0	4,8,8	1.26	0
2	DTT	A	1717	-	7,7,7	0.86	0	4,8,8	0.48	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	B	1717	-	-	0/8/8/8	-
2	DTT	A	1717	-	-	1/8/8/8	-

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 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1717	DTT	2	0
2	A	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, 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	689/714 (96%)	0.37	67 (9%)	13 14	11, 20, 56, 63	0
1	B	689/714 (96%)	0.48	85 (12%)	8 8	11, 20, 57, 62	0
All	All	1378/1428 (96%)	0.42	152 (11%)	10 10	11, 20, 57, 63	0

All (152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	343	LEU	9.9
1	B	343	LEU	8.8
1	A	342	PRO	8.7
1	A	112	VAL	8.1
1	B	118	ALA	8.0
1	B	342	PRO	7.9
1	B	556	LEU	7.8
1	B	112	VAL	7.3
1	A	115	GLY	7.3
1	A	337	LEU	7.2
1	B	561	PHE	7.0
1	B	334	ALA	7.0
1	A	557	HIS	6.9
1	B	115	GLY	6.9
1	B	120	SER	6.9
1	B	552	VAL	6.9
1	A	124	THR	6.9
1	A	109	SER	6.8
1	B	107	THR	6.7
1	A	118	ALA	6.7
1	A	346	PRO	6.7
1	B	121	HIS	6.6
1	B	558	PRO	6.5
1	B	716	CYS	6.5

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Mol	Chain	Res	Type	RSRZ
1	A	341	ASP	6.3
1	A	107	THR	6.3
1	A	106	GLY	6.2
1	A	113	THR	6.2
1	B	124	THR	6.2
1	A	110	TYR	6.1
1	B	110	TYR	6.1
1	B	127	GLY	6.0
1	A	338	HIS	6.0
1	A	108	ASP	5.9
1	B	122	ARG	5.9
1	A	552	VAL	5.8
1	A	558	PRO	5.7
1	B	551	GLY	5.6
1	A	550	MET	5.5
1	A	551	GLY	5.4
1	B	117	GLY	5.4
1	A	121	HIS	5.4
1	A	120	SER	5.3
1	B	126	GLN	5.3
1	B	116	PHE	5.2
1	B	119	THR	5.2
1	B	346	PRO	5.1
1	B	557	HIS	5.1
1	B	337	LEU	5.1
1	A	119	THR	5.1
1	A	549	THR	4.9
1	A	339	GLU	4.8
1	B	559	SER	4.8
1	B	549	THR	4.8
1	B	550	MET	4.8
1	A	716	CYS	4.8
1	A	111	GLY	4.8
1	B	114	THR	4.8
1	A	122	ARG	4.6
1	A	116	PHE	4.6
1	B	347	LYS	4.6
1	A	340	MET	4.6
1	B	554	GLY	4.6
1	A	344	GLN	4.6
1	A	345	LYS	4.6
1	A	554	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	340	MET	4.5
1	B	715	ILE	4.5
1	A	127	GLY	4.4
1	B	106	GLY	4.4
1	B	341	ASP	4.4
1	B	339	GLU	4.3
1	B	125	LYS	4.3
1	B	338	HIS	4.3
1	B	383	ASP	4.2
1	A	123	ARG	4.2
1	B	333	ALA	4.1
1	A	559	SER	4.0
1	B	123	ARG	4.0
1	B	111	GLY	3.9
1	B	113	THR	3.8
1	B	348	GLN	3.8
1	B	332	LYS	3.8
1	B	344	GLN	3.8
1	A	556	LEU	3.7
1	B	109	SER	3.7
1	A	245	GLY	3.5
1	B	560	ARG	3.5
1	A	114	THR	3.5
1	B	553	ASN	3.5
1	B	153	HIS	3.5
1	A	306	HIS	3.4
1	A	126	GLN	3.4
1	B	611	LEU	3.3
1	B	606	ASP	3.3
1	A	117	GLY	3.3
1	B	335	GLN	3.3
1	B	555	GLU	3.2
1	A	336	LYS	3.2
1	B	245	GLY	3.2
1	A	125	LYS	3.2
1	A	611	LEU	3.2
1	A	333	ALA	3.2
1	B	548	LEU	3.1
1	B	108	ASP	3.1
1	B	345	LYS	3.1
1	A	334	ALA	3.1
1	A	105	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	331	VAL	3.0
1	B	486	HIS	3.0
1	A	544	ALA	3.0
1	A	560	ARG	2.8
1	B	246	GLY	2.8
1	B	542	SER	2.8
1	B	260	ASN	2.8
1	A	260	ASN	2.8
1	B	336	LYS	2.7
1	A	335	GLN	2.7
1	B	77	GLY	2.7
1	B	105	LYS	2.6
1	A	297	LYS	2.6
1	B	590	MET	2.6
1	B	644	GLY	2.6
1	B	547	VAL	2.6
1	A	103	MET	2.5
1	B	104	ASN	2.5
1	A	606	ASP	2.5
1	A	303	HIS	2.5
1	B	311	HIS	2.5
1	A	332	LYS	2.5
1	A	347	LYS	2.5
1	A	605	GLY	2.5
1	A	553	ASN	2.4
1	B	25	GLU	2.4
1	B	128	GLY	2.4
1	B	562	CYS	2.4
1	B	601	ALA	2.3
1	A	561	PHE	2.3
1	B	609	ARG	2.3
1	A	610	ASN	2.3
1	B	382	ASN	2.2
1	B	629	LEU	2.2
1	B	75	ARG	2.2
1	A	546	ARG	2.1
1	B	74	ALA	2.1
1	B	76	ASP	2.1
1	A	651	ARG	2.1
1	A	310	HIS	2.1
1	B	616	PHE	2.1
1	A	555	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	647	ALA	2.0
1	B	613	THR	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, 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
1	MDO	A	203	13/14	0.92	0.07	14,15,20,27	0
1	MDO	B	203	13/14	0.95	0.07	13,15,19,29	0

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	B	1717	8/8	0.88	0.14	34,40,42,43	0
2	DTT	A	1717	8/8	0.93	0.11	30,35,37,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.