



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 06:50 PM GMT

PDB ID : 2O1X
Title : 1-deoxy-D-xylulose 5-phosphate synthase (DXS) from *Deinococcus radiodurans*
Authors : Xiang, S.; Usunow, G.; Lange, G.; Busch, M.; Tong, L.
Deposited on : 2006-11-29
Resolution : 2.90 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

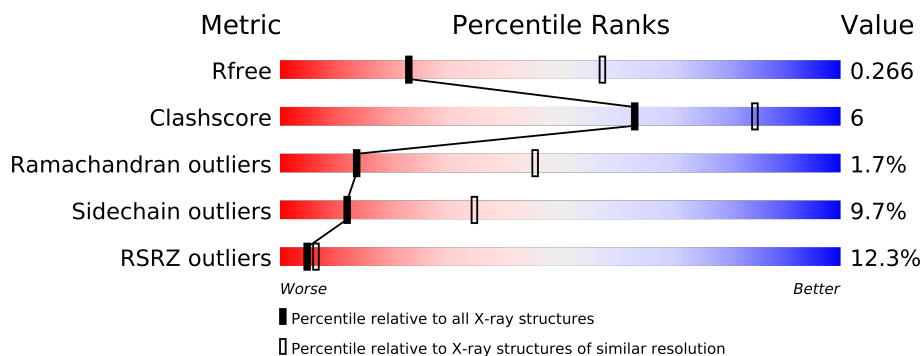
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.90 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}	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	629	
1	B	629	
1	C	629	
1	D	629	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	MG	B	2002	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16910 atoms, of which 0 are hydrogen and 0 are deuterium.

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 1-deoxy-D-xylulose-5-phosphatesynthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	578	Total	C	N	O	S	0	0	0
			4362	2753	771	821	17			
1	B	579	Total	C	N	O	S	0	0	0
			4376	2761	775	823	17			
1	C	538	Total	C	N	O	S	0	0	0
			4063	2558	724	766	15			
1	D	530	Total	C	N	O	S	0	0	0
			4001	2521	715	750	15			

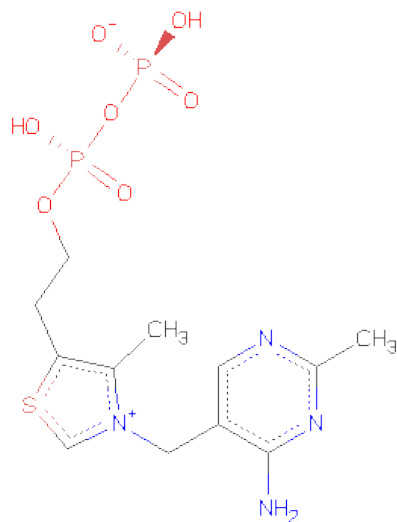
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	130	THR	ALA	ENGINEERED	UNP Q9RUB5
B	130	THR	ALA	ENGINEERED	UNP Q9RUB5
C	130	THR	ALA	ENGINEERED	UNP Q9RUB5
D	130	THR	ALA	ENGINEERED	UNP Q9RUB5

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is THIAMIN DIPHOSPHATE (three-letter code: TDP) (formula: C₁₂H₁₈N₄O₇P₂S).

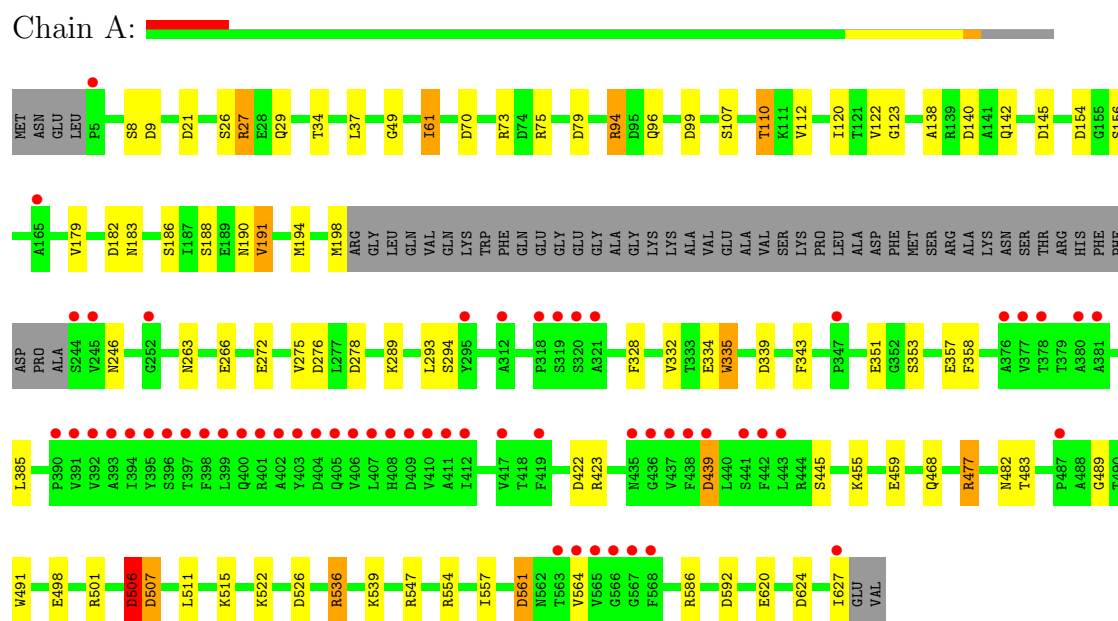


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	B	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	C	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	D	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

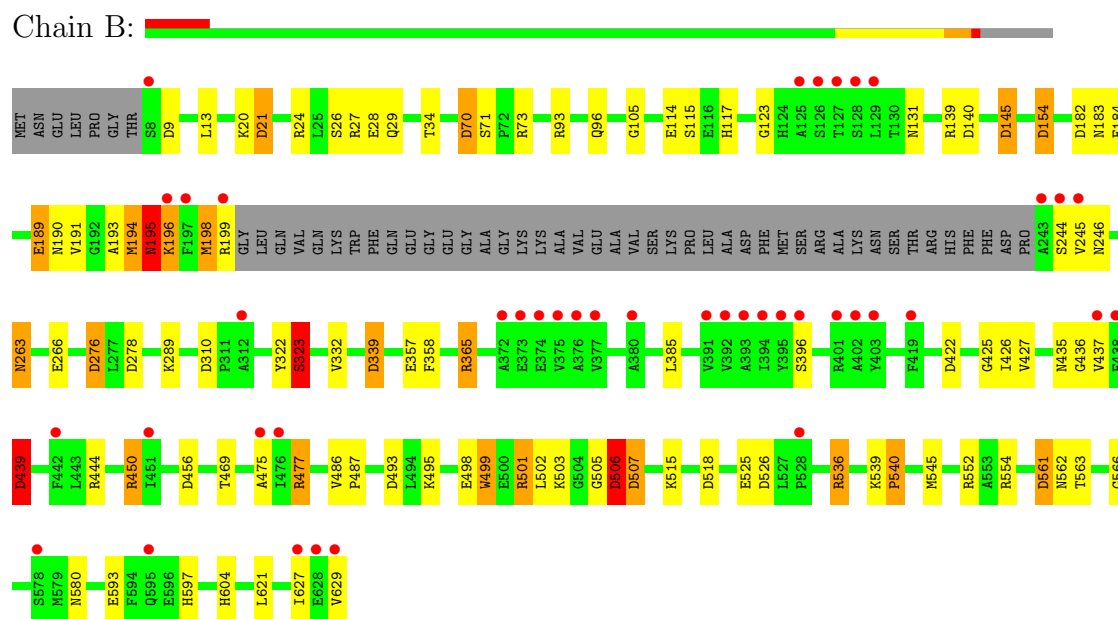
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: 1-deoxy-D-xylulose-5-phosphatesynthase



- Molecule 1: 1-deoxy-D-xylulose-5-phosphatesynthase



Chain C:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.26Å 154.06Å 124.88Å 90.00° 98.91° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 29.25 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.4 (30.00-2.90) 97.4 (29.25-2.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.44 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.209 , 0.272 0.207 , 0.266	Depositor DCC
R_{free} test set	3204 reflections (5.09%)	DCC
Wilson B-factor (Å ²)	40.7	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 1.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 62969 reflections	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	16910	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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: MG, TDP

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	0.53	0/4452	0.85	19/6049 (0.3%)
1	B	0.53	0/4465	0.87	16/6066 (0.3%)
1	C	0.43	0/4139	0.80	18/5621 (0.3%)
1	D	0.83	6/4076 (0.1%)	0.80	15/5534 (0.3%)
All	All	0.60	6/17132 (0.0%)	0.83	68/23270 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	36	GLU	CD-OE2	28.08	1.56	1.25
1	D	628	GLU	CD-OE1	23.04	1.50	1.25
1	D	628	GLU	CD-OE2	18.05	1.45	1.25
1	D	36	GLU	CD-OE1	16.34	1.43	1.25
1	D	28	GLU	CD-OE2	9.40	1.35	1.25
1	D	28	GLU	CD-OE1	7.49	1.33	1.25

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	182	ASP	CB-CG-OD2	7.46	125.02	118.30
1	D	561	ASP	CB-CG-OD2	7.41	124.97	118.30
1	B	310	ASP	CB-CG-OD2	7.27	124.84	118.30
1	A	154	ASP	CB-CG-OD2	7.21	124.79	118.30
1	C	422	ASP	CB-CG-OD2	7.20	124.78	118.30
1	A	182	ASP	CB-CG-OD2	7.19	124.77	118.30
1	A	439	ASP	CB-CG-OD2	6.92	124.52	118.30
1	C	518	ASP	CB-CG-OD2	6.81	124.43	118.30
1	D	422	ASP	CB-CG-OD2	6.81	124.43	118.30
1	B	422	ASP	CB-CG-OD2	6.64	124.28	118.30
1	B	154	ASP	CB-CG-OD2	6.53	124.18	118.30
1	B	278	ASP	CB-CG-OD2	6.49	124.14	118.30
1	B	561	ASP	CB-CG-OD2	6.30	123.97	118.30
1	B	493	ASP	CB-CG-OD2	6.25	123.92	118.30
1	D	182	ASP	CB-CG-OD2	6.22	123.90	118.30
1	C	409	ASP	CB-CG-OD2	6.21	123.89	118.30
1	A	21	ASP	CB-CG-OD2	6.08	123.77	118.30
1	B	540	PRO	N-CD-CG	-6.07	94.09	103.20
1	A	276	ASP	CB-CG-OD2	6.07	123.76	118.30
1	A	145	ASP	CB-CG-OD2	6.07	123.76	118.30
1	C	278	ASP	CB-CG-OD2	6.07	123.76	118.30
1	D	339	ASP	CB-CG-OD2	5.97	123.68	118.30
1	A	278	ASP	CB-CG-OD2	5.96	123.66	118.30
1	A	79	ASP	CB-CG-OD2	5.95	123.66	118.30
1	C	404	ASP	CB-CG-OD2	5.93	123.64	118.30
1	A	339	ASP	CB-CG-OD2	5.90	123.61	118.30
1	D	154	ASP	CB-CG-OD2	5.87	123.59	118.30
1	A	624	ASP	CB-CG-OD2	5.84	123.56	118.30
1	A	9	ASP	CB-CG-OD2	5.75	123.48	118.30
1	A	140	ASP	CB-CG-OD2	5.72	123.45	118.30
1	C	507	ASP	CB-CG-OD2	5.72	123.45	118.30
1	B	145	ASP	CB-CG-OD2	5.72	123.44	118.30
1	C	506	ASP	CB-CG-OD2	5.71	123.44	118.30
1	D	60	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	422	ASP	CB-CG-OD2	5.61	123.35	118.30
1	D	36	GLU	CG-CD-OE2	-5.61	107.08	118.30
1	D	276	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	99	ASP	CB-CG-OD2	5.58	123.33	118.30
1	B	21	ASP	CB-CG-OD2	5.58	123.32	118.30
1	B	506	ASP	CB-CG-OD2	5.54	123.28	118.30
1	C	74	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	561	ASP	CB-CG-OD2	5.51	123.26	118.30
1	C	95	ASP	CB-CG-OD2	5.45	123.21	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	561	ASP	CB-CG-OD2	5.45	123.21	118.30
1	C	339	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	70	ASP	CB-CG-OD2	5.42	123.17	118.30
1	A	592	ASP	CB-CG-OD2	5.38	123.15	118.30
1	C	624	ASP	CB-CG-OD2	5.34	123.11	118.30
1	C	21	ASP	CB-CG-OD2	5.32	123.09	118.30
1	B	339	ASP	CB-CG-OD2	5.31	123.08	118.30
1	C	260	ASP	CB-CG-OD2	5.30	123.07	118.30
1	C	526	ASP	CB-CG-OD2	5.28	123.05	118.30
1	D	610	ASP	CB-CG-OD2	5.27	123.05	118.30
1	D	36	GLU	OE1-CD-OE2	5.26	129.62	123.30
1	C	171	ASP	CB-CG-OD2	5.23	123.00	118.30
1	C	9	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	518	ASP	CB-CG-OD2	5.21	122.99	118.30
1	B	456	ASP	CB-CG-OD2	5.18	122.97	118.30
1	C	276	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	70	ASP	CB-CG-OD2	5.17	122.95	118.30
1	B	276	ASP	CB-CG-OD2	5.15	122.93	118.30
1	A	506	ASP	CB-CG-OD2	5.11	122.90	118.30
1	D	507	ASP	CB-CG-OD2	5.08	122.87	118.30
1	D	70	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	526	ASP	CB-CG-OD2	5.07	122.86	118.30
1	D	74	ASP	CB-CG-OD2	5.05	122.85	118.30
1	D	99	ASP	CB-CG-OD2	5.05	122.85	118.30
1	D	506	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	191	VAL	Peptide
1	B	539	LYS	Peptide
1	C	438	PHE	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4362	0	0	18	0
1	B	4376	0	0	31	0
1	C	4063	0	0	16	0
1	D	4001	0	0	24	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	26	0	16	1	0
3	B	26	0	16	3	0
3	C	26	0	16	1	0
3	D	26	0	16	2	0
All	All	16910	0	64	94	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (94) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:1003:TDP:C2	3:C:1003:TDP:H2	0.97	1.49
3:B:1002:TDP:H2	3:B:1002:TDP:C2	0.97	1.47
3:D:1004:TDP:H2	3:D:1004:TDP:C2	0.97	1.47
3:A:1001:TDP:H2	3:A:1001:TDP:C2	0.97	1.46
1:B:139:ARG:NH1	1:B:140:ASP:OD1	2.23	0.72
1:B:71:SER:OG	1:B:117:HIS:CD2	2.42	0.72
1:B:498:GLU:O	1:B:536:ARG:NH1	2.24	0.70
1:C:535:ALA:O	1:C:537:PHE:N	2.25	0.70
1:A:110:THR:CG2	1:A:120:ILE:O	2.40	0.70
1:C:402:ALA:CA	1:C:405:GLN:NE2	2.56	0.69
1:D:186:SER:OG	1:D:189:GLU:O	2.11	0.68
1:C:75:ARG:NH1	1:C:75:ARG:CG	2.56	0.68
1:D:439:ASP:OD2	1:D:477:ARG:CD	2.43	0.65
1:D:246:ASN:O	1:D:248:PHE:N	2.30	0.64
1:A:439:ASP:OD2	1:A:477:ARG:NH1	2.30	0.63
1:B:339:ASP:O	1:B:365:ARG:NH2	2.32	0.63
1:D:93:ARG:NH1	1:D:114:GLU:OE2	2.32	0.63
1:A:586:ARG:NH2	1:A:620:GLU:OE1	2.33	0.62
1:A:27:ARG:NH2	1:A:272:GLU:OE1	2.35	0.60
1:B:194:MET:O	1:B:196:LYS:N	2.34	0.60
1:B:198:MET:O	1:B:198:MET:CG	2.50	0.59
1:A:498:GLU:O	1:A:536:ARG:NH1	2.35	0.59
1:A:335:TRP:CZ3	1:A:468:GLN:CG	2.86	0.58
1:B:322:TYR:O	1:B:323:SER:CB	2.52	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:554:ARG:NH2	1:B:621:LEU:O	2.36	0.58
1:B:365:ARG:NH1	1:B:365:ARG:CG	2.67	0.57
1:B:506:ASP:O	1:B:507:ASP:CB	2.53	0.57
1:B:21:ASP:OD1	1:B:24:ARG:NH1	2.37	0.56
1:C:328:PHE:O	1:C:331:ALA:N	2.38	0.56
1:B:477:ARG:NH2	1:B:561:ASP:O	2.39	0.55
1:D:414:HIS:CE1	1:D:450:ARG:NH2	2.77	0.53
1:D:183:ASN:ND2	3:D:1004:TDP:O21	2.42	0.53
1:B:425:GLY:N	1:B:436:GLY:O	2.42	0.53
1:B:26:SER:N	1:B:29:GLN:NE2	2.58	0.52
1:D:499:TRP:CD1	1:D:533:VAL:CG1	2.92	0.52
1:A:506:ASP:O	1:A:507:ASP:CB	2.57	0.52
1:B:105:GLY:O	1:B:597:HIS:CE1	2.63	0.52
1:A:138:ALA:O	1:A:142:GLN:CG	2.59	0.51
1:D:246:ASN:C	1:D:248:PHE:N	2.64	0.51
1:B:469:THR:O	1:B:469:THR:CG2	2.60	0.49
1:B:499:TRP:CD1	1:B:545:MET:SD	3.05	0.49
1:B:486:VAL:CG1	1:B:487:PRO:CD	2.91	0.49
1:B:444:ARG:NH1	1:B:566:GLY:O	2.45	0.48
1:C:552:ARG:NH1	1:C:552:ARG:CG	2.74	0.48
1:C:499:TRP:CD1	1:C:535:ALA:O	2.66	0.48
1:B:154:ASP:O	1:B:195:ASN:ND2	2.47	0.48
1:B:501:ARG:NH2	1:B:505:GLY:O	2.46	0.48
1:B:93:ARG:NH1	1:B:114:GLU:OE2	2.46	0.48
1:C:186:SER:O	1:C:187:ILE:C	2.51	0.48
1:D:477:ARG:NH2	1:D:561:ASP:O	2.47	0.48
1:D:552:ARG:NH1	1:D:552:ARG:CG	2.77	0.48
1:C:590:ILE:N	1:C:590:ILE:CD1	2.77	0.48
1:B:183:ASN:ND2	3:B:1002:TDP:O22	2.48	0.47
1:B:193:ALA:O	1:B:194:MET:C	2.53	0.47
1:D:370:GLY:O	1:D:372:ALA:N	2.47	0.47
1:A:477:ARG:NH2	1:A:561:ASP:O	2.48	0.47
1:B:450:ARG:O	1:B:475:ALA:N	2.47	0.47
1:C:453:LEU:N	1:C:536:ARG:O	2.48	0.47
1:C:270:LEU:O	1:C:274:LEU:N	2.48	0.47
1:D:44:VAL:O	1:D:44:VAL:CG1	2.63	0.47
1:D:582:HIS:N	1:D:582:HIS:ND1	2.62	0.47
1:D:75:ARG:CG	1:D:75:ARG:NH1	2.78	0.46
3:B:1002:TDP:H2	3:B:1002:TDP:H4'2	1.80	0.46
1:D:466:TYR:O	1:D:470:HIS:CD2	2.68	0.46
1:C:174:ARG:NE	1:C:174:ARG:N	2.64	0.46
1:D:79:ASP:OD1	1:D:126:SER:N	2.49	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:396:SER:OG	1:B:439:ASP:OD2	2.34	0.46
1:D:147:HIS:ND1	1:D:275:VAL:O	2.50	0.45
1:B:437:VAL:O	1:B:437:VAL:CG1	2.63	0.45
1:A:26:SER:N	1:A:29:GLN:NE2	2.63	0.45
1:A:358:PHE:C	1:A:358:PHE:CD2	2.90	0.44
1:B:358:PHE:C	1:B:358:PHE:CD2	2.91	0.44
1:D:165:ALA:O	1:D:169:ILE:N	2.51	0.44
1:C:188:SER:OG	1:C:350:ARG:NH1	2.50	0.44
1:C:466:TYR:O	1:C:470:HIS:CD2	2.71	0.44
1:C:79:ASP:O	1:C:83:GLN:NE2	2.51	0.43
1:D:246:ASN:O	1:D:247:PRO:C	2.56	0.43
1:B:561:ASP:OD2	1:B:604:HIS:CE1	2.72	0.42
1:C:402:ALA:C	1:C:405:GLN:NE2	2.73	0.42
1:A:335:TRP:CD1	1:A:491:TRP:CH2	3.08	0.42
1:D:611:ALA:CB	1:D:612:PRO:CD	2.97	0.42
1:A:334:GLU:OE1	1:A:489:GLY:N	2.53	0.42
1:D:91:THR:OG1	1:D:93:ARG:NH2	2.52	0.42
1:B:427:VAL:N	1:B:435:ASN:ND2	2.68	0.42
1:A:455:LYS:N	1:A:459:GLU:OE2	2.53	0.41
1:D:439:ASP:CB	1:D:477:ARG:NH1	2.83	0.41
1:D:591:PRO:O	1:D:593:GLU:N	2.53	0.41
1:A:94:ARG:NH1	1:A:94:ARG:CG	2.83	0.41
1:A:293:LEU:O	1:A:294:SER:C	2.59	0.41
1:B:263:ASN:C	1:B:263:ASN:ND2	2.74	0.41
1:A:511:LEU:N	1:A:557:ILE:O	2.54	0.40
1:A:61:ILE:CD1	1:A:179:VAL:CG1	2.99	0.40
1:C:423:ARG:CD	1:C:480:ARG:CG	2.99	0.40
1:D:334:GLU:OE1	1:D:489:GLY:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	574/629 (91%)	536 (93%)	34 (6%)	4 (1%)	30 72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	575/629 (91%)	531 (92%)	32 (6%)	12 (2%)	11	39
1	C	532/629 (85%)	473 (89%)	48 (9%)	11 (2%)	11	39
1	D	524/629 (83%)	470 (90%)	44 (8%)	10 (2%)	12	42
All	All	2205/2516 (88%)	2010 (91%)	158 (7%)	37 (2%)	14	45

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	507	ASP
1	B	194	MET
1	B	195	ASN
1	B	244	SER
1	B	439	ASP
1	B	540	PRO
1	C	439	ASP
1	D	247	PRO
1	D	439	ASP
1	D	536	ARG
1	D	628	GLU
1	A	49	GLY
1	B	507	ASP
1	C	187	ILE
1	C	322	TYR
1	B	323	SER
1	C	175	LYS
1	C	506	ASP
1	D	189	GLU
1	D	371	ILE
1	D	525	GLU
1	B	189	GLU
1	B	196	LYS
1	B	525	GLU
1	C	123	GLY
1	C	173	GLY
1	D	188	SER
1	A	328	PHE
1	C	51	HIS
1	C	507	ASP
1	C	580	ASN
1	B	246	ASN
1	B	123	GLY

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Mol	Chain	Res	Type
1	D	123	GLY
1	D	187	ILE
1	A	123	GLY
1	C	258	PRO

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	452/493 (92%)	404 (89%)	48 (11%)	10	28
1	B	453/493 (92%)	404 (89%)	49 (11%)	9	27
1	C	422/493 (86%)	380 (90%)	42 (10%)	11	32
1	D	414/493 (84%)	384 (93%)	30 (7%)	21	51
All	All	1741/1972 (88%)	1572 (90%)	169 (10%)	12	35

All (169) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	27	ARG
1	A	34	THR
1	A	37	LEU
1	A	61	ILE
1	A	73	ARG
1	A	75	ARG
1	A	94	ARG
1	A	96	GLN
1	A	107	SER
1	A	110	THR
1	A	112	VAL
1	A	122	VAL
1	A	156	SER
1	A	183	ASN
1	A	186	SER
1	A	188	SER
1	A	190	ASN

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Mol	Chain	Res	Type
1	A	191	VAL
1	A	194	MET
1	A	198	MET
1	A	246	ASN
1	A	263	ASN
1	A	266	GLU
1	A	275	VAL
1	A	289	LYS
1	A	332	VAL
1	A	335	TRP
1	A	343	PHE
1	A	351	GLU
1	A	353	SER
1	A	357	GLU
1	A	385	LEU
1	A	423	ARG
1	A	445	SER
1	A	477	ARG
1	A	482	ASN
1	A	483	THR
1	A	501	ARG
1	A	506	ASP
1	A	515	LYS
1	A	522	LYS
1	A	536	ARG
1	A	539	LYS
1	A	547	ARG
1	A	554	ARG
1	A	564	VAL
1	A	627	ILE
1	B	9	ASP
1	B	13	LEU
1	B	20	LYS
1	B	27	ARG
1	B	28	GLU
1	B	34	THR
1	B	70	ASP
1	B	73	ARG
1	B	96	GLN
1	B	115	SER
1	B	131	ASN
1	B	145	ASP

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Mol	Chain	Res	Type
1	B	184	GLU
1	B	189	GLU
1	B	190	ASN
1	B	191	VAL
1	B	195	ASN
1	B	198	MET
1	B	199	ARG
1	B	245	VAL
1	B	263	ASN
1	B	266	GLU
1	B	276	ASP
1	B	289	LYS
1	B	323	SER
1	B	332	VAL
1	B	357	GLU
1	B	365	ARG
1	B	385	LEU
1	B	426	ILE
1	B	439	ASP
1	B	450	ARG
1	B	477	ARG
1	B	495	LYS
1	B	499	TRP
1	B	501	ARG
1	B	502	LEU
1	B	503	LYS
1	B	506	ASP
1	B	515	LYS
1	B	526	ASP
1	B	536	ARG
1	B	552	ARG
1	B	562	ASN
1	B	563	THR
1	B	580	ASN
1	B	593	GLU
1	B	627	ILE
1	B	629	VAL
1	C	13	LEU
1	C	20	LYS
1	C	74	ASP
1	C	75	ARG
1	C	83	GLN

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Mol	Chain	Res	Type
1	C	122	VAL
1	C	130	THR
1	C	131	ASN
1	C	137	LEU
1	C	168	THR
1	C	174	ARG
1	C	181	ASN
1	C	185	MET
1	C	251	MET
1	C	259	VAL
1	C	263	ASN
1	C	269	TRP
1	C	332	VAL
1	C	351	GLU
1	C	357	GLU
1	C	385	LEU
1	C	397	THR
1	C	405	GLN
1	C	421	ILE
1	C	426	ILE
1	C	433	THR
1	C	434	HIS
1	C	437	VAL
1	C	439	ASP
1	C	450	ARG
1	C	494	LEU
1	C	511	LEU
1	C	515	LYS
1	C	543	GLU
1	C	552	ARG
1	C	554	ARG
1	C	565	VAL
1	C	580	ASN
1	C	581	LEU
1	C	585	VAL
1	C	610	ASP
1	C	624	ASP
1	D	17	HIS
1	D	22	LEU
1	D	28	GLU
1	D	34	THR
1	D	71	SER

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Mol	Chain	Res	Type
1	D	75	ARG
1	D	96	GLN
1	D	113	SER
1	D	122	VAL
1	D	144	LYS
1	D	146	PHE
1	D	185	MET
1	D	186	SER
1	D	190	ASN
1	D	191	VAL
1	D	259	VAL
1	D	266	GLU
1	D	273	ARG
1	D	330	GLU
1	D	332	VAL
1	D	351	GLU
1	D	357	GLU
1	D	360	ARG
1	D	385	LEU
1	D	397	THR
1	D	482	ASN
1	D	507	ASP
1	D	536	ARG
1	D	539	LYS
1	D	552	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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
3	TDP	A	1001	2	27,27,27	1.98	9 (33%)	40,40,40	1.95	12 (30%)
3	TDP	B	1002	2	27,27,27	1.70	7 (25%)	40,40,40	1.99	10 (25%)
3	TDP	C	1003	2	27,27,27	2.06	9 (33%)	40,40,40	2.50	12 (30%)
3	TDP	D	1004	2	27,27,27	1.84	9 (33%)	40,40,40	2.15	14 (35%)

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
3	TDP	A	1001	2	-	0/17/17/17	0/2/2/2
3	TDP	B	1002	2	-	0/17/17/17	0/2/2/2
3	TDP	C	1003	2	-	0/17/17/17	0/2/2/2
3	TDP	D	1004	2	-	0/17/17/17	0/2/2/2

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	TDP	P2-O21	4.54	1.65	1.50
3	B	1002	TDP	P2-O22	4.46	1.65	1.50
3	A	1001	TDP	P2-O22	4.13	1.64	1.50
3	D	1004	TDP	P2-O22	3.99	1.64	1.50
3	A	1001	TDP	C5-S1	-3.81	1.70	1.73
3	C	1003	TDP	P2-O21	3.80	1.62	1.50
3	C	1003	TDP	C5A-C5	3.79	1.56	1.51
3	C	1003	TDP	P2-O22	3.71	1.63	1.50
3	C	1003	TDP	C5-C4	3.68	1.41	1.36
3	C	1003	TDP	P1-O11	3.49	1.66	1.59
3	D	1004	TDP	P1-O12	3.49	1.64	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	TDP	P1-O12	3.45	1.64	1.51
3	D	1004	TDP	P2-O21	3.42	1.61	1.50
3	D	1004	TDP	C5-C4	3.31	1.40	1.36
3	B	1002	TDP	C4-N3	-3.10	1.36	1.39
3	B	1002	TDP	P2-O21	3.02	1.60	1.50
3	C	1003	TDP	P2-O11	2.88	1.67	1.60
3	B	1002	TDP	P1-O12	2.84	1.62	1.51
3	A	1001	TDP	C2-S1	2.63	1.77	1.68
3	C	1003	TDP	P1-O12	2.61	1.61	1.51
3	A	1001	TDP	P1-O11	2.45	1.64	1.59
3	D	1004	TDP	C5-S1	-2.43	1.71	1.73
3	A	1001	TDP	C5-C4	2.41	1.39	1.36
3	D	1004	TDP	C5A-C5	2.34	1.54	1.51
3	D	1004	TDP	C4A-C4	2.33	1.54	1.49
3	A	1001	TDP	C4-N3	-2.25	1.37	1.39
3	B	1002	TDP	C5-C4	2.25	1.39	1.36
3	C	1003	TDP	C4A-C4	2.23	1.54	1.49
3	D	1004	TDP	C4-N3	-2.21	1.37	1.39
3	B	1002	TDP	C2-S1	2.21	1.75	1.68
3	D	1004	TDP	C35-C5'	2.14	1.56	1.51
3	C	1003	TDP	C35-C5'	2.07	1.55	1.51
3	B	1002	TDP	C5-S1	-2.04	1.72	1.73
3	A	1001	TDP	P2-O23	-2.00	1.46	1.55

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1003	TDP	C2-S1-C5	7.90	96.91	91.63
3	C	1003	TDP	C4-C5-S1	-6.47	104.64	109.93
3	D	1004	TDP	C2-S1-C5	6.12	95.73	91.63
3	C	1003	TDP	C5A-C5-C4	5.28	131.28	127.44
3	B	1002	TDP	C2-S1-C5	4.82	94.85	91.63
3	A	1001	TDP	C2-S1-C5	4.58	94.69	91.63
3	D	1004	TDP	C4-C5-S1	-4.32	106.40	109.93
3	B	1002	TDP	S1-C2-N3	-4.28	106.21	112.62
3	A	1001	TDP	S1-C2-N3	-4.25	106.25	112.62
3	C	1003	TDP	S1-C2-N3	-4.08	106.51	112.62
3	C	1003	TDP	C5-C4-N3	3.92	115.50	107.53
3	D	1004	TDP	S1-C2-N3	-3.85	106.86	112.62
3	A	1001	TDP	C4A-C4-C5	-3.71	119.83	129.10
3	B	1002	TDP	C2A-C2'-N1'	3.66	121.38	117.02
3	B	1002	TDP	C5-C4-N3	3.59	114.83	107.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	TDP	C5-C4-N3	3.49	114.63	107.53
3	D	1004	TDP	C5A-C5-C4	3.48	129.97	127.44
3	D	1004	TDP	C2A-C2'-N1'	3.43	121.10	117.02
3	D	1004	TDP	C5-C4-N3	3.37	114.38	107.53
3	B	1002	TDP	C4-C5-S1	-3.36	107.18	109.93
3	C	1003	TDP	C4A-C4-C5	-3.33	120.78	129.10
3	B	1002	TDP	N1'-C2'-N3'	-3.20	119.88	125.65
3	B	1002	TDP	C6'-N1'-C2'	3.14	121.20	115.68
3	C	1003	TDP	O23-P2-O11	3.12	114.23	104.29
3	A	1001	TDP	N1'-C2'-N3'	-3.10	120.05	125.65
3	D	1004	TDP	N1'-C2'-N3'	-3.00	120.24	125.65
3	A	1001	TDP	C5A-C5-C4	2.98	129.61	127.44
3	D	1004	TDP	C4A-C4-C5	-2.95	121.75	129.10
3	C	1003	TDP	C35-N3-C2	-2.93	118.83	125.05
3	B	1002	TDP	C4A-C4-C5	-2.90	121.86	129.10
3	C	1003	TDP	C6'-N1'-C2'	2.84	120.67	115.68
3	C	1003	TDP	N1'-C2'-N3'	-2.84	120.53	125.65
3	D	1004	TDP	O23-P2-O11	2.82	113.27	104.29
3	B	1002	TDP	C5A-C5-C4	2.79	129.47	127.44
3	A	1001	TDP	C6'-N1'-C2'	2.74	120.50	115.68
3	A	1001	TDP	C35-C5'-C6'	-2.66	115.42	120.73
3	D	1004	TDP	P2-O11-P1	-2.60	121.80	132.95
3	A	1001	TDP	C4-C5-S1	-2.57	107.83	109.93
3	C	1003	TDP	C2A-C2'-N1'	2.56	120.07	117.02
3	D	1004	TDP	O22-P2-O21	-2.49	102.63	114.56
3	D	1004	TDP	C6'-N1'-C2'	2.46	120.00	115.68
3	B	1002	TDP	C2-N3-C4	2.33	116.91	110.82
3	A	1001	TDP	C4A-C4-N3	2.31	125.54	122.53
3	D	1004	TDP	C2-N3-C4	2.23	116.63	110.82
3	A	1001	TDP	C2-N3-C4	2.20	116.56	110.82
3	C	1003	TDP	C2-N3-C4	2.15	116.42	110.82
3	D	1004	TDP	C35-N3-C2	-2.15	120.49	125.05
3	A	1001	TDP	C35-N3-C2	-2.05	120.70	125.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	578/629 (91%)	0.71	58 (10%) 8 10	-5, 10, 34, 53	0
1	B	579/629 (92%)	0.22	42 (7%) 15 18	-3, 11, 39, 75	0
1	C	538/629 (85%)	0.77	87 (16%) 2 3	6, 65, 139, 191	0
1	D	530/629 (84%)	0.75	88 (16%) 2 3	7, 60, 133, 175	0
All	All	2225/2516 (88%)	0.61	275 (12%) 5 6	-5, 24, 121, 191	0

All (275) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	128	SER	24.6
1	B	127	THR	23.9
1	A	566	GLY	22.6
1	B	392	VAL	21.5
1	A	396	SER	21.2
1	A	391	VAL	20.6
1	A	392	VAL	18.9
1	A	436	GLY	17.9
1	A	564	VAL	16.9
1	B	375	VAL	16.3
1	B	376	ALA	15.5
1	A	410	VAL	15.2
1	A	393	ALA	15.0
1	B	403	TYR	14.5
1	A	398	PHE	14.3
1	B	393	ALA	14.3
1	A	377	VAL	14.0
1	A	399	LEU	13.9
1	A	411	ALA	13.9
1	A	397	THR	13.9
1	A	395	TYR	13.7

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Mol	Chain	Res	Type	RSRZ
1	A	394	ILE	13.6
1	A	403	TYR	13.6
1	A	565	VAL	13.4
1	B	394	ILE	13.3
1	A	406	VAL	13.3
1	A	407	LEU	13.1
1	A	438	PHE	12.9
1	A	412	ILE	12.7
1	A	563	THR	12.6
1	A	442	PHE	12.6
1	B	129	LEU	12.3
1	A	380	ALA	12.1
1	B	126	SER	11.9
1	B	377	VAL	11.7
1	B	402	ALA	11.4
1	B	395	TYR	11.0
1	A	443	LEU	10.7
1	A	402	ALA	10.3
1	A	381	ALA	10.2
1	B	396	SER	9.5
1	D	46	SER	9.3
1	A	409	ASP	9.0
1	A	437	VAL	8.9
1	A	390	PRO	8.8
1	A	405	GLN	8.5
1	A	376	ALA	8.5
1	C	627	ILE	8.1
1	A	419	PHE	8.0
1	C	321	ALA	7.3
1	B	438	PHE	7.1
1	A	347	PRO	7.0
1	D	49	GLY	6.5
1	A	567	GLY	6.2
1	B	125	ALA	5.8
1	D	45	CYS	5.7
1	C	48	GLY	5.5
1	B	437	VAL	5.5
1	C	7	THR	5.5
1	C	628	GLU	5.4
1	B	373	GLU	5.4
1	C	555	ALA	5.3
1	A	404	ASP	5.3

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Mol	Chain	Res	Type	RSRZ
1	C	528	PRO	5.2
1	C	9	ASP	5.1
1	A	439	ASP	5.1
1	C	104	GLY	5.1
1	D	622	GLY	5.1
1	D	484	ALA	5.1
1	B	391	VAL	5.0
1	B	629	VAL	5.0
1	A	408	HIS	4.9
1	B	244	SER	4.9
1	D	254	ARG	4.9
1	D	245	VAL	4.8
1	C	15	GLN	4.7
1	C	8	SER	4.7
1	D	147	HIS	4.5
1	D	190	ASN	4.5
1	D	48	GLY	4.4
1	D	32	ALA	4.4
1	C	67	TYR	4.4
1	D	96	GLN	4.2
1	D	62	ILE	4.2
1	D	42	VAL	4.2
1	C	544	GLU	4.2
1	B	451	ILE	4.2
1	A	401	ARG	4.1
1	C	11	PRO	4.1
1	C	288	THR	4.1
1	A	312	ALA	4.1
1	C	145	ASP	4.1
1	D	185	MET	4.1
1	C	17	HIS	4.1
1	C	47	ARG	4.0
1	A	165	ALA	4.0
1	A	245	VAL	4.0
1	B	401	ARG	4.0
1	D	321	ALA	4.0
1	D	263	ASN	3.9
1	D	290	GLY	3.9
1	B	8	SER	3.9
1	C	25	LEU	3.9
1	B	374	GLU	3.9
1	C	615	ARG	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	554	ARG	3.9
1	D	188	SER	3.9
1	C	52	LEU	3.9
1	D	24	ARG	3.8
1	A	244	SER	3.8
1	C	245	VAL	3.8
1	B	380	ALA	3.8
1	D	104	GLY	3.8
1	B	243	ALA	3.8
1	C	24	ARG	3.8
1	D	98	ALA	3.7
1	D	145	ASP	3.7
1	C	508	VAL	3.6
1	B	442	PHE	3.6
1	C	59	VAL	3.6
1	D	257	GLY	3.6
1	C	246	ASN	3.6
1	C	144	LYS	3.6
1	C	62	ILE	3.6
1	B	628	GLU	3.5
1	B	199	ARG	3.4
1	A	400	GLN	3.4
1	D	44	VAL	3.4
1	D	247	PRO	3.4
1	D	76	ILE	3.4
1	D	615	ARG	3.3
1	C	267	LEU	3.3
1	C	526	ASP	3.3
1	C	70	ASP	3.3
1	D	146	PHE	3.3
1	D	20	LYS	3.2
1	B	245	VAL	3.2
1	C	73	ARG	3.2
1	D	627	ILE	3.2
1	A	568	PHE	3.2
1	A	378	THR	3.2
1	D	250	ALA	3.2
1	D	523	ALA	3.2
1	D	17	HIS	3.1
1	C	290	GLY	3.1
1	C	618	LEU	3.1
1	B	372	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	269	TRP	3.1
1	C	20	LYS	3.1
1	D	258	PRO	3.1
1	D	47	ARG	3.0
1	D	624	ASP	3.0
1	A	435	ASN	3.0
1	D	580	ASN	3.0
1	C	269	TRP	3.0
1	D	486	VAL	3.0
1	C	84	ALA	3.0
1	C	249	ALA	3.0
1	A	627	ILE	3.0
1	B	595	GLN	3.0
1	C	33	LEU	2.9
1	C	185	MET	2.9
1	D	598	ALA	2.9
1	B	578	SER	2.9
1	D	481	GLY	2.9
1	C	323	SER	2.8
1	D	144	LYS	2.8
1	D	255	TYR	2.8
1	B	196	LYS	2.8
1	C	257	GLY	2.8
1	D	31	PRO	2.8
1	C	322	TYR	2.8
1	C	263	ASN	2.8
1	C	16	ILE	2.8
1	C	46	SER	2.8
1	D	86	ALA	2.8
1	C	77	LEU	2.8
1	D	78	PHE	2.8
1	D	354	GLY	2.8
1	A	441	SER	2.8
1	D	151	VAL	2.8
1	D	521	LEU	2.8
1	C	43	ARG	2.7
1	D	508	VAL	2.7
1	C	85	TYR	2.7
1	C	612	PRO	2.7
1	D	95	ASP	2.7
1	D	629	VAL	2.7
1	B	419	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	73	ARG	2.6
1	D	29	GLN	2.6
1	C	175	LYS	2.6
1	D	252	GLY	2.6
1	D	265	GLN	2.6
1	C	45	CYS	2.6
1	D	100	ILE	2.6
1	D	26	SER	2.6
1	D	530	VAL	2.6
1	A	321	ALA	2.5
1	D	35	GLU	2.5
1	A	319	SER	2.5
1	C	53	ALA	2.5
1	D	61	ILE	2.5
1	C	76	ILE	2.4
1	C	35	GLU	2.4
1	D	555	ALA	2.4
1	D	81	GLY	2.4
1	D	85	TYR	2.4
1	D	256	VAL	2.4
1	C	184	GLU	2.4
1	D	620	GLU	2.4
1	C	78	PHE	2.4
1	C	98	ALA	2.4
1	C	277	LEU	2.3
1	C	286	VAL	2.3
1	C	147	HIS	2.3
1	C	61	ILE	2.3
1	C	247	PRO	2.3
1	D	544	GLU	2.3
1	D	628	GLU	2.3
1	B	476	ILE	2.3
1	C	143	GLY	2.3
1	A	417	VAL	2.3
1	A	318	PRO	2.3
1	C	626	PRO	2.3
1	C	484	ALA	2.3
1	D	64	ALA	2.3
1	D	52	LEU	2.3
1	B	475	ALA	2.3
1	D	92	GLY	2.3
1	D	471	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	105	GLY	2.3
1	C	429	ALA	2.3
1	B	197	PHE	2.3
1	B	528	PRO	2.2
1	C	287	THR	2.2
1	C	507	ASP	2.2
1	D	253	VAL	2.2
1	C	282	ILE	2.2
1	A	320	SER	2.2
1	A	295	TYR	2.2
1	D	25	LEU	2.2
1	C	506	ASP	2.2
1	C	187	ILE	2.2
1	C	509	VAL	2.2
1	D	509	VAL	2.2
1	B	312	ALA	2.2
1	C	552	ARG	2.2
1	D	50	LEU	2.2
1	D	189	GLU	2.2
1	C	281	THR	2.2
1	C	86	ALA	2.1
1	C	87	HIS	2.1
1	A	487	PRO	2.1
1	C	186	SER	2.1
1	D	360	ARG	2.1
1	C	116	GLU	2.1
1	C	42	VAL	2.1
1	C	117	HIS	2.1
1	A	252	GLY	2.1
1	D	99	ASP	2.1
1	D	27	ARG	2.1
1	C	289	LYS	2.1
1	C	579	MET	2.1
1	D	84	ALA	2.1
1	D	276	ASP	2.0
1	D	249	ALA	2.0
1	D	23	LYS	2.0
1	D	41	ILE	2.0
1	C	66	HIS	2.0
1	A	5	PRO	2.0
1	D	28	GLU	2.0
1	B	627	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	32	ALA	2.0
1	C	619	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	MG	B	2002	1/1	0.22	2.76	8,8,8,8	0
2	MG	A	2001	1/1	0.21	1.58	9,9,9,9	0
3	TDP	B	1002	26/26	0.13	-0.40	2,3,4,6	0
3	TDP	A	1001	26/26	0.12	-0.43	2,2,4,5	0
3	TDP	D	1004	26/26	0.18	-0.49	40,44,48,48	0
3	TDP	C	1003	26/26	0.15	-1.11	50,50,52,53	0
2	MG	D	2004	1/1	0.10	-1.55	35,35,35,35	0
2	MG	C	2003	1/1	0.11	-2.02	33,33,33,33	0

6.5 Other polymers ⓘ

There are no such residues in this entry.