



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:24 AM GMT

PDB ID : 3D4N
Title : Crystal Structure of Human 11-beta-HydroxysteroidDehydrogenase (HSD1)
in Complex with Sulfonamide Inhibitor
Authors : Wang, Z.; Liu, J.; Sudom, A.; Walker, N.P.
Deposited on : 2008-05-14
Resolution : 2.50 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>

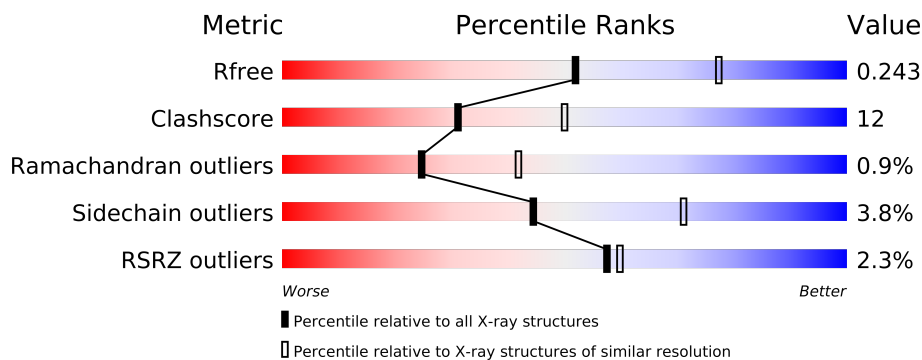
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.50 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	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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	286	
1	B	286	
1	C	286	
1	D	286	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8585 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 Corticosteroid 11-beta-dehydrogenase isozyme 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	7	0
			2023	1289	342	377	15			
1	B	265	Total	C	N	O	S	0	6	0
			2050	1310	344	380	16			
1	C	260	Total	C	N	O	S	0	2	0
			2001	1276	339	371	15			
1	D	261	Total	C	N	O	S	0	9	0
			2032	1295	341	379	17			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MET	-	EXPRESSION TAG	UNP P28845
A	8	LYS	-	EXPRESSION TAG	UNP P28845
A	9	HIS	-	EXPRESSION TAG	UNP P28845
A	10	GLN	-	EXPRESSION TAG	UNP P28845
A	11	HIS	-	EXPRESSION TAG	UNP P28845
A	12	GLN	-	EXPRESSION TAG	UNP P28845
A	13	HIS	-	EXPRESSION TAG	UNP P28845
A	14	GLN	-	EXPRESSION TAG	UNP P28845
A	15	HIS	-	EXPRESSION TAG	UNP P28845
A	16	GLN	-	EXPRESSION TAG	UNP P28845
A	17	HIS	-	EXPRESSION TAG	UNP P28845
A	18	GLN	-	EXPRESSION TAG	UNP P28845
A	19	HIS	-	EXPRESSION TAG	UNP P28845
A	20	GLN	-	EXPRESSION TAG	UNP P28845
A	21	GLN	-	EXPRESSION TAG	UNP P28845
A	22	PRO	-	EXPRESSION TAG	UNP P28845
A	23	LEU	-	EXPRESSION TAG	UNP P28845
A	272	SER	CYS	ENGINEERED	UNP P28845
B	7	MET	-	EXPRESSION TAG	UNP P28845
B	8	LYS	-	EXPRESSION TAG	UNP P28845
B	9	HIS	-	EXPRESSION TAG	UNP P28845

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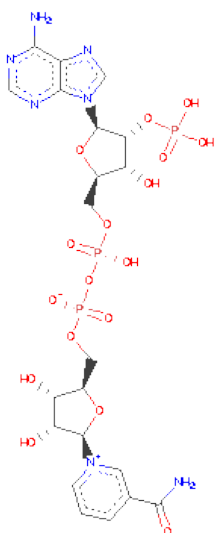
Chain	Residue	Modelled	Actual	Comment	Reference
B	10	GLN	-	EXPRESSION TAG	UNP P28845
B	11	HIS	-	EXPRESSION TAG	UNP P28845
B	12	GLN	-	EXPRESSION TAG	UNP P28845
B	13	HIS	-	EXPRESSION TAG	UNP P28845
B	14	GLN	-	EXPRESSION TAG	UNP P28845
B	15	HIS	-	EXPRESSION TAG	UNP P28845
B	16	GLN	-	EXPRESSION TAG	UNP P28845
B	17	HIS	-	EXPRESSION TAG	UNP P28845
B	18	GLN	-	EXPRESSION TAG	UNP P28845
B	19	HIS	-	EXPRESSION TAG	UNP P28845
B	20	GLN	-	EXPRESSION TAG	UNP P28845
B	21	GLN	-	EXPRESSION TAG	UNP P28845
B	22	PRO	-	EXPRESSION TAG	UNP P28845
B	23	LEU	-	EXPRESSION TAG	UNP P28845
B	272	SER	CYS	ENGINEERED	UNP P28845
C	7	MET	-	EXPRESSION TAG	UNP P28845
C	8	LYS	-	EXPRESSION TAG	UNP P28845
C	9	HIS	-	EXPRESSION TAG	UNP P28845
C	10	GLN	-	EXPRESSION TAG	UNP P28845
C	11	HIS	-	EXPRESSION TAG	UNP P28845
C	12	GLN	-	EXPRESSION TAG	UNP P28845
C	13	HIS	-	EXPRESSION TAG	UNP P28845
C	14	GLN	-	EXPRESSION TAG	UNP P28845
C	15	HIS	-	EXPRESSION TAG	UNP P28845
C	16	GLN	-	EXPRESSION TAG	UNP P28845
C	17	HIS	-	EXPRESSION TAG	UNP P28845
C	18	GLN	-	EXPRESSION TAG	UNP P28845
C	19	HIS	-	EXPRESSION TAG	UNP P28845
C	20	GLN	-	EXPRESSION TAG	UNP P28845
C	21	GLN	-	EXPRESSION TAG	UNP P28845
C	22	PRO	-	EXPRESSION TAG	UNP P28845
C	23	LEU	-	EXPRESSION TAG	UNP P28845
C	272	SER	CYS	ENGINEERED	UNP P28845
D	7	MET	-	EXPRESSION TAG	UNP P28845
D	8	LYS	-	EXPRESSION TAG	UNP P28845
D	9	HIS	-	EXPRESSION TAG	UNP P28845
D	10	GLN	-	EXPRESSION TAG	UNP P28845
D	11	HIS	-	EXPRESSION TAG	UNP P28845
D	12	GLN	-	EXPRESSION TAG	UNP P28845
D	13	HIS	-	EXPRESSION TAG	UNP P28845
D	14	GLN	-	EXPRESSION TAG	UNP P28845
D	15	HIS	-	EXPRESSION TAG	UNP P28845

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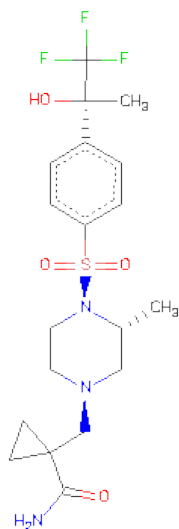
Chain	Residue	Modelled	Actual	Comment	Reference
D	16	GLN	-	EXPRESSION TAG	UNP P28845
D	17	HIS	-	EXPRESSION TAG	UNP P28845
D	18	GLN	-	EXPRESSION TAG	UNP P28845
D	19	HIS	-	EXPRESSION TAG	UNP P28845
D	20	GLN	-	EXPRESSION TAG	UNP P28845
D	21	GLN	-	EXPRESSION TAG	UNP P28845
D	22	PRO	-	EXPRESSION TAG	UNP P28845
D	23	LEU	-	EXPRESSION TAG	UNP P28845
D	272	SER	CYS	ENGINEERED	UNP P28845

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDEPHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 1-{[(3R)-3-METHYL-4-({4-[(1S)-2,2,2-TRIFLUORO-1-HYDROXY-1-METHYLETHYL]PHENYL}SULFONYL)PIPERAZIN-1-YL]METHYL}CYCLOPROPANECARBOXAMIDE (three-letter code: D4N) (formula: $C_{19}H_{26}F_3N_3O_4S$).



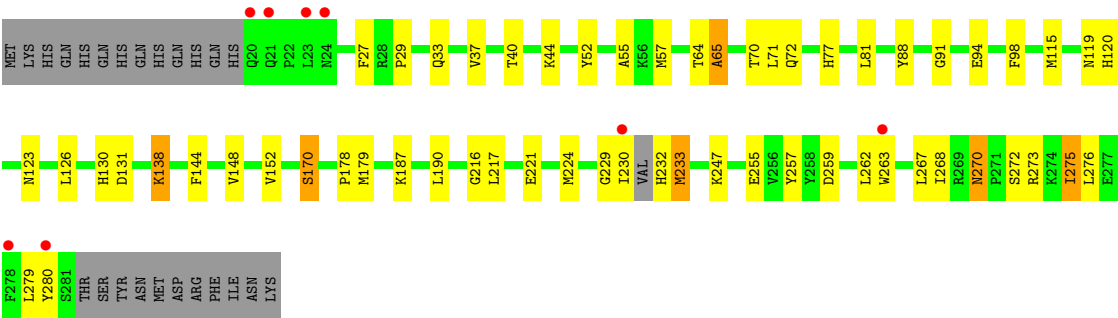
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	S	0	0
			30	19	3	3	4	1		
3	B	1	Total	C	F	N	O	S	0	0
			30	19	3	3	4	1		
3	C	1	Total	C	F	N	O	S	0	0
			30	19	3	3	4	1		
3	D	1	Total	C	F	N	O	S	0	0
			30	19	3	3	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	52	Total	O	0	0
			52	52		
4	B	48	Total	O	0	0
			48	48		
4	C	47	Total	O	0	0
			47	47		
4	D	20	Total	O	0	0
			20	20		

● Molecule 1: Corticosteroid 11-beta-dehydrogenaseisozyme 1

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.62Å 153.76Å 73.91Å 90.00° 93.11° 90.00°	Depositor
Resolution (Å)	76.92 – 2.50 56.54 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.5 (76.92-2.50) 93.5 (56.54-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.83 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, R_{free}	0.227 , 0.259 0.221 , 0.243	Depositor DCC
R_{free} test set	2050 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	31.0	Xtriage
Anisotropy	0.732	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 18.1	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 40748 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8585	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, D4N

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	0.30	0/2089	0.51	0/2820
1	B	0.30	0/2113	0.52	0/2854
1	C	0.31	0/2042	0.49	0/2755
1	D	0.28	0/2104	0.48	0/2837
All	All	0.30	0/8348	0.50	0/11266

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2023	0	2072	64	0
1	B	2050	0	2106	59	0
1	C	2001	0	2046	41	0
1	D	2032	0	2075	50	0
2	A	48	0	25	1	0
2	B	48	0	25	2	0
2	C	48	0	25	3	0
2	D	48	0	25	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	30	0	26	0	0
3	B	30	0	26	0	0
3	C	30	0	26	0	0
3	D	30	0	26	0	0
4	A	52	0	0	0	0
4	B	48	0	0	0	0
4	C	47	0	0	0	0
4	D	20	0	0	0	0
All	All	8585	0	8503	198	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 12.

All (198) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:230:ILE:O	1:A:231:VAL:HG22	1.27	1.28
1:D:229:GLY:O	1:D:230:ILE:HG12	1.22	1.26
1:A:230:ILE:O	1:A:231:VAL:CG2	1.97	1.13
1:A:227:VAL:HG23	1:A:228:SER:H	1.10	1.09
1:D:230:ILE:O	1:D:232:HIS:HB3	1.55	1.04
1:C:233:MET:SD	1:C:233:MET:O	2.24	0.95
1:D:229:GLY:O	1:D:230:ILE:CG1	2.15	0.95
1:C:60:HIS:HD1	1:C:85:SER:HG	1.19	0.90
1:A:230:ILE:C	1:A:231:VAL:CG2	2.38	0.88
1:A:109:LEU:HD23	1:A:109:LEU:C	1.95	0.87
1:C:272:SER:O	1:C:276:LEU:HD12	1.76	0.85
1:A:227:VAL:HG23	1:A:228:SER:N	1.91	0.84
1:A:129:PHE:HB3	1:B:197[B]:ILE:HD11	1.57	0.84
1:B:105:GLN:O	1:B:109:LEU:HD13	1.79	0.81
1:B:261:SER:O	1:B:265:THR:HG23	1.82	0.79
1:A:230:ILE:C	1:A:231:VAL:HG23	2.02	0.79
1:A:130:HIS:C	1:A:132:ASP:H	1.90	0.74
1:A:109:LEU:HD23	1:A:109:LEU:O	1.87	0.73
1:A:40:THR:OG1	1:A:120:HIS:HD2	1.71	0.73
1:D:270:ASN:HD22	1:D:270:ASN:C	1.91	0.73
1:C:56:LYS:HE3	1:C:81:LEU:HD22	1.70	0.72
1:B:230:ILE:O	1:B:231:VAL:CG2	2.38	0.72
1:A:227:VAL:O	1:A:228:SER:C	2.31	0.69
1:D:94:GLU:OE2	1:D:138:LYS:NZ	2.25	0.69
1:B:122:THR:O	1:B:124:THR:HG22	1.92	0.68
1:D:217:LEU:HD21	1:D:224:MET:HE3	1.76	0.68
1:B:171:LEU:HD22	1:B:268:ILE:HD13	1.75	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:227:VAL:CG2	1:A:228:SER:H	1.96	0.67
1:C:270:ASN:C	1:C:270:ASN:HD22	1.98	0.66
1:A:109:LEU:CD2	1:A:109:LEU:C	2.64	0.65
1:A:276:LEU:HB3	1:A:280:TYR:CE1	2.32	0.65
1:D:229:GLY:C	1:D:230:ILE:HG12	2.12	0.65
1:C:216:GLY:HA3	1:C:259:ASP:OD2	1.98	0.62
1:D:230:ILE:O	1:D:232:HIS:CB	2.42	0.62
1:C:93:MET:HG3	1:C:120:HIS:CE1	2.35	0.61
1:B:216:GLY:HA3	1:B:259:ASP:OD2	2.00	0.61
1:D:263:TRP:O	1:D:267:LEU:HB2	1.99	0.61
1:B:194:PHE:CD2	1:B:197[A]:ILE:HD11	2.36	0.61
1:B:272:SER:O	1:B:276:LEU:HG	2.01	0.60
1:B:228:SER:O	1:B:230:ILE:HG13	2.01	0.60
1:B:230:ILE:O	1:B:231:VAL:HG22	1.99	0.60
1:B:230:ILE:C	1:B:231:VAL:HG23	2.21	0.60
1:B:273:ARG:HA	1:B:276:LEU:HD12	1.84	0.59
1:D:276:LEU:HB3	1:D:280:TYR:CE1	2.38	0.59
1:C:270:ASN:HD21	1:C:272:SER:HB2	1.66	0.59
1:A:126:LEU:HD11	1:A:227:VAL:HG12	1.84	0.58
1:B:119:ASN:HD22	1:B:168:VAL:HG21	1.69	0.58
1:B:228:SER:O	1:B:230:ILE:N	2.36	0.58
1:C:77:HIS:CD2	1:C:81:LEU:HD11	2.39	0.57
1:A:28:ARG:O	1:A:31:MET:HG3	2.05	0.57
1:A:130:HIS:C	1:A:132:ASP:N	2.58	0.57
1:B:178:PRO:O	1:B:179[B]:MET:HB2	2.04	0.57
1:D:217:LEU:HD21	1:D:224:MET:CE	2.34	0.56
1:C:267:LEU:HB3	1:D:276:LEU:HD21	1.88	0.56
1:B:266:LEU:O	1:B:269:ARG:HG2	2.05	0.56
1:A:276:LEU:HD21	1:B:267:LEU:HB3	1.88	0.56
1:A:91:GLY:HA3	1:A:98:PHE:CZ	2.41	0.55
1:B:40:THR:OG1	1:B:120:HIS:HD2	1.89	0.55
1:C:23:LEU:C	1:C:25:GLU:H	2.10	0.55
1:D:178:PRO:O	1:D:179[B]:MET:HB2	2.06	0.55
1:D:40:THR:OG1	1:D:120:HIS:HD2	1.90	0.55
1:B:199:LYS:O	1:B:203:VAL:HG12	2.06	0.54
1:B:64:THR:O	1:B:65:ALA:HB2	2.07	0.54
1:C:131:ASP:HB3	1:D:152:VAL:HG13	1.88	0.54
1:C:137:ARG:O	1:C:141:GLU:HG3	2.07	0.54
1:A:129:PHE:CB	1:B:197[B]:ILE:HD11	2.32	0.54
1:B:228:SER:C	1:B:230:ILE:H	2.10	0.54
1:B:155:LEU:HB3	1:B:156:PRO:HD3	1.88	0.53
1:D:130:HIS:O	1:D:131:ASP:OD1	2.26	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:270:ASN:C	1:C:270:ASN:ND2	2.60	0.53
1:D:270:ASN:C	1:D:270:ASN:ND2	2.60	0.53
1:D:40:THR:HA	1:D:64:THR:HG22	1.90	0.53
1:B:129:PHE:CZ	1:B:131:ASP:HA	2.43	0.53
1:C:171:LEU:HD22	1:C:268:ILE:HD13	1.90	0.53
1:D:44:LYS:HG2	2:D:4:NAP:H3B	1.91	0.53
1:B:230:ILE:C	1:B:231:VAL:CG2	2.77	0.53
1:C:64:THR:HB	1:C:102:PHE:CE1	2.44	0.52
1:B:230:ILE:O	1:B:231:VAL:HG23	2.06	0.52
1:C:194:PHE:HA	1:C:197:ILE:HG12	1.91	0.52
1:B:42:ALA:HB3	1:B:63:VAL:HB	1.91	0.52
1:D:29:PRO:HB3	1:D:57:MET:HG2	1.92	0.52
1:A:91:GLY:HA3	1:A:98:PHE:CE1	2.44	0.52
1:B:148:VAL:HG22	1:B:193:PHE:CE1	2.45	0.52
1:A:71:LEU:HD13	1:A:88:TYR:HB2	1.91	0.51
1:A:119:ASN:HD22	1:A:168:VAL:HG21	1.76	0.51
1:D:272:SER:O	1:D:275:ILE:HB	2.10	0.51
1:D:275:ILE:HG22	1:D:276:LEU:N	2.25	0.51
1:A:276:LEU:HB3	1:A:280:TYR:HE1	1.75	0.51
1:B:144:PHE:CD2	1:B:145[B]:LEU:HD12	2.45	0.51
1:A:267:LEU:HB3	1:B:276:LEU:HD21	1.93	0.50
1:B:140:MET:HE3	1:B:144:PHE:HB3	1.93	0.50
1:A:37:VAL:HG22	1:A:115:MET:HB3	1.93	0.50
1:D:221:GLU:OE1	1:D:221:GLU:HA	2.12	0.50
1:C:126:LEU:HD11	1:C:227:VAL:HG12	1.94	0.50
1:B:270:ASN:HD22	1:B:271:PRO:HD2	1.75	0.50
1:A:267:LEU:HB3	1:B:276:LEU:CD2	2.42	0.50
1:B:119:ASN:ND2	2:B:2:NAP:H4D	2.27	0.49
1:B:126:LEU:HD22	1:B:179[B]:MET:HB3	1.93	0.49
1:B:104:ALA:O	1:B:108:LYS:HG3	2.12	0.49
1:D:255:GLU:OE2	1:D:257:TYR:OH	2.20	0.49
1:C:131:ASP:HB3	1:D:152:VAL:CG1	2.43	0.49
1:A:69:GLU:O	1:A:72:GLN:HB2	2.13	0.49
1:D:270:ASN:ND2	1:D:273:ARG:H	2.11	0.49
1:D:72:GLN:OE1	1:D:88:TYR:CE2	2.66	0.48
1:C:270:ASN:HA	1:C:271:PRO:HD2	1.64	0.48
1:C:272:SER:O	1:C:276:LEU:CD1	2.56	0.48
1:A:227:VAL:CG2	1:A:228:SER:N	2.64	0.48
1:A:126:LEU:HD22	1:A:179:MET:HB2	1.96	0.48
1:C:139:SER:O	1:C:143:ASN:HB2	2.14	0.48
1:C:88:TYR:CD1	1:C:88:TYR:C	2.87	0.48
1:D:170:SER:HB3	2:D:4:NAP:H5N	1.96	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:40:THR:O	1:A:119:ASN:HB3	2.14	0.47
1:C:276:LEU:HD21	1:D:267:LEU:HB3	1.95	0.47
1:C:178:PRO:O	1:C:179:MET:HB2	2.14	0.47
1:A:263:TRP:O	1:A:267:LEU:HG	2.14	0.47
1:A:171:LEU:C	1:A:173:GLY:H	2.16	0.47
1:A:193:PHE:HB2	1:B:185:ALA:HB2	1.97	0.47
1:D:72:GLN:OE1	1:D:88:TYR:HE2	1.98	0.47
1:C:49:GLU:OE1	1:C:238:LYS:HE2	2.15	0.47
1:D:233:MET:H	1:D:233:MET:HE3	1.78	0.47
1:A:126:LEU:HD12	1:A:226:ALA:O	2.14	0.47
1:C:213:CYS:SG	1:C:245:ILE:HG23	2.54	0.47
1:A:273:ARG:O	1:A:277:GLU:HG3	2.15	0.47
1:D:216:GLY:HA3	1:D:259:ASP:OD2	2.14	0.47
1:C:26:GLU:H	1:C:26:GLU:HG2	1.60	0.47
1:B:93:MET:HG3	1:B:120:HIS:CE1	2.50	0.46
1:B:194:PHE:HA	1:B:197[A]:ILE:HG12	1.96	0.46
1:D:270:ASN:HD21	1:D:272:SER:HB2	1.80	0.46
1:A:131:ASP:O	1:A:133:ILE:N	2.49	0.46
1:B:53:HIS:O	1:B:57:MET:HG3	2.15	0.46
1:B:93:MET:HG2	2:B:2:NAP:H2A	1.97	0.46
1:D:217:LEU:CD2	1:D:224:MET:HE3	2.44	0.46
1:A:120:HIS:HE1	1:A:146:SER:OG	1.98	0.45
1:B:227:VAL:O	1:B:228:SER:C	2.53	0.45
1:C:270:ASN:ND2	1:C:273:ARG:H	2.15	0.45
1:A:261:SER:O	1:A:265:THR:HG22	2.17	0.45
1:D:233:MET:H	1:D:233:MET:CE	2.29	0.45
1:D:52:TYR:O	1:D:55:ALA:HB3	2.17	0.45
1:B:217:LEU:O	1:B:218:ILE:HD13	2.17	0.45
1:B:67[B]:SER:HB2	1:B:70:THR:OG1	2.17	0.44
1:A:239:GLU:CD	1:A:239:GLU:H	2.19	0.44
1:A:131:ASP:OD2	1:B:152:VAL:HG13	2.17	0.44
1:A:180:VAL:HG23	1:A:184:SER:HG	1.83	0.44
1:D:187:LYS:O	1:D:190:LEU:HB2	2.18	0.44
1:B:263:TRP:CE3	1:D:279:LEU:HD13	2.54	0.43
1:B:30:GLU:H	1:B:30:GLU:CD	2.22	0.43
1:C:276:LEU:HD22	1:D:268:ILE:HD12	2.01	0.43
1:C:194:PHE:CD2	1:C:197:ILE:HD11	2.54	0.43
1:A:224:MET:HA	1:A:224:MET:CE	2.48	0.43
1:B:279:LEU:HD13	1:D:263:TRP:CE3	2.54	0.43
1:B:255:GLU:OE2	1:B:257:TYR:OH	2.29	0.43
1:A:148:VAL:O	1:A:152:VAL:HG23	2.19	0.43
1:D:224:MET:HE2	1:D:224:MET:HA	2.01	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:131:ASP:C	1:D:131:ASP:OD1	2.57	0.43
1:D:37:VAL:HG22	1:D:115:MET:HB3	2.01	0.43
1:A:139:SER:O	1:A:143:ASN:HB2	2.18	0.43
1:D:77:HIS:CE1	1:D:81:LEU:HD11	2.54	0.43
1:A:169:SER:HB2	1:A:212:LEU:HD11	2.00	0.43
1:A:178:PRO:C	1:A:179:MET:HG2	2.38	0.43
1:C:169:SER:N	1:C:213:CYS:O	2.50	0.43
1:A:75:VAL:HG13	1:A:86:ALA:O	2.19	0.42
1:D:91:GLY:HA3	1:D:98:PHE:CZ	2.54	0.42
1:A:215:LEU:HD11	1:A:245:ILE:HD11	2.01	0.42
1:A:119:ASN:ND2	2:A:1:NAP:H4D	2.35	0.42
1:B:141:GLU:OE1	1:B:145[A]:LEU:HD23	2.19	0.42
1:B:204[B]:SER:OG	1:B:206:VAL:HG23	2.19	0.42
1:A:126:LEU:HD22	1:A:179:MET:CB	2.49	0.42
1:C:121:ILE:HG12	2:C:3:NAP:H3D	2.00	0.42
1:C:119:ASN:ND2	2:C:3:NAP:H4D	2.35	0.42
1:B:144:PHE:HD2	1:B:145[B]:LEU:HD12	1.83	0.42
1:C:91:GLY:HA3	1:C:98:PHE:CZ	2.54	0.42
1:C:40:THR:OG1	1:C:120:HIS:HD2	2.03	0.42
1:A:262:LEU:HA	1:A:265:THR:HG23	2.01	0.41
1:C:46:ILE:HD11	1:C:218:ILE:HG13	2.02	0.41
1:A:133:ILE:HD13	1:B:149:VAL:HG22	2.02	0.41
1:A:39:VAL:HG12	1:A:42:ALA:HB2	2.02	0.41
1:A:218:ILE:O	1:A:220:THR:N	2.52	0.41
1:B:261:SER:OG	1:B:263:TRP:HB2	2.20	0.41
1:B:87:HIS:CB	1:B:109:LEU:HD23	2.50	0.41
1:D:126:LEU:HB3	1:D:179[B]:MET:SD	2.60	0.41
1:A:140:MET:HE3	1:A:144:PHE:HB3	2.03	0.41
1:A:175:VAL:HG12	1:B:273:ARG:HG3	2.02	0.41
1:C:224:MET:HA	1:C:224:MET:CE	2.50	0.41
1:D:64:THR:O	1:D:65:ALA:HB2	2.20	0.41
1:A:171:LEU:C	1:A:173:GLY:N	2.74	0.41
1:A:177:TYR:HB3	1:A:178:PRO:HD2	2.02	0.41
1:A:276:LEU:HD22	1:A:280:TYR:OH	2.20	0.41
1:D:144:PHE:O	1:D:148:VAL:HG23	2.21	0.41
1:B:194:PHE:HD2	1:B:197[A]:ILE:HD11	1.82	0.41
1:B:197[B]:ILE:HD13	1:B:200:GLU:OE2	2.20	0.41
1:A:196:SER:O	1:A:200:GLU:HG3	2.21	0.40
1:A:270:ASN:C	1:A:270:ASN:ND2	2.74	0.40
1:D:27:PHE:CD2	1:D:247:LYS:HG2	2.56	0.40
1:A:87:HIS:CD2	1:A:109:LEU:HD11	2.56	0.40
1:C:198:ARG:HA	1:C:210:ILE:HD12	2.03	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:271:PRO:O	1:C:272:SER:C	2.58	0.40
1:C:93:MET:HG2	2:C:3:NAP:H2A	2.03	0.40
1:D:71:LEU:HD13	1:D:88:TYR:HB2	2.04	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	264/286 (92%)	247 (94%)	14 (5%)	3 (1%)	21	34
1	B	269/286 (94%)	250 (93%)	16 (6%)	3 (1%)	21	34
1	C	258/286 (90%)	238 (92%)	18 (7%)	2 (1%)	27	46
1	D	266/286 (93%)	252 (95%)	13 (5%)	1 (0%)	43	66
All	All	1057/1144 (92%)	987 (93%)	61 (6%)	9 (1%)	25	42

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	ASP
1	A	231	VAL
1	B	229	GLY
1	A	219	ASP
1	B	65	ALA
1	D	65	ALA
1	C	24	ASN
1	C	22	PRO
1	B	231	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	226/243 (93%)	221 (98%)	5 (2%)	64	88
1	B	228/243 (94%)	219 (96%)	9 (4%)	43	70
1	C	219/243 (90%)	210 (96%)	9 (4%)	41	67
1	D	227/243 (93%)	217 (96%)	10 (4%)	39	64
All	All	900/972 (93%)	867 (96%)	33 (4%)	44	72

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ARG
1	A	170	SER
1	A	231	VAL
1	A	265	THR
1	A	270	ASN
1	B	124	THR
1	B	138	LYS
1	B	170	SER
1	B	203	VAL
1	B	205	ARG
1	B	234	GLN
1	B	265	THR
1	B	268	ILE
1	B	270	ASN
1	C	26	GLU
1	C	44	LYS
1	C	131	ASP
1	C	199	LYS
1	C	205	ARG
1	C	233	MET
1	C	260	SER
1	C	265	THR
1	C	270	ASN
1	D	33	GLN
1	D	70	THR
1	D	119	ASN
1	D	123	ASN
1	D	138	LYS
1	D	170	SER
1	D	233	MET

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Mol	Chain	Res	Type
1	D	262	LEU
1	D	270	ASN
1	D	275	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	24	ASN
1	A	87	HIS
1	A	119	ASN
1	A	120	HIS
1	A	135	HIS
1	A	270	ASN
1	B	119	ASN
1	B	120	HIS
1	B	135	HIS
1	B	270	ASN
1	C	24	ASN
1	C	87	HIS
1	C	119	ASN
1	C	120	HIS
1	C	135	HIS
1	C	270	ASN
1	D	120	HIS
1	D	253	GLN
1	D	270	ASN

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

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAP	A	1	-	52,52,52	1.32	3 (5%)	80,80,80	1.61	9 (11%)
3	D4N	A	293	-	32,32,32	2.03	1 (3%)	52,52,52	2.27	13 (25%)
2	NAP	B	2	-	52,52,52	1.32	3 (5%)	80,80,80	1.78	10 (12%)
3	D4N	B	293	-	32,32,32	1.93	1 (3%)	52,52,52	1.97	10 (19%)
3	D4N	C	293	-	32,32,32	1.97	1 (3%)	52,52,52	1.99	12 (23%)
2	NAP	C	3	-	52,52,52	1.33	3 (5%)	80,80,80	1.67	9 (11%)
3	D4N	D	293	-	32,32,32	1.96	1 (3%)	52,52,52	1.98	11 (21%)
2	NAP	D	4	-	52,52,52	1.35	3 (5%)	80,80,80	1.64	9 (11%)

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	NAP	A	1	-	-	0/35/67/67	0/3/5/5
3	D4N	A	293	-	-	0/38/55/55	0/2/3/3
2	NAP	B	2	-	-	0/35/67/67	0/3/5/5
3	D4N	B	293	-	-	0/38/55/55	0/2/3/3
3	D4N	C	293	-	-	0/38/55/55	0/2/3/3
2	NAP	C	3	-	-	0/35/67/67	0/3/5/5
3	D4N	D	293	-	-	0/38/55/55	0/2/3/3
2	NAP	D	4	-	-	0/35/67/67	0/3/5/5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	293	D4N	C11-S14	-10.80	1.60	1.76
3	D	293	D4N	C11-S14	-10.40	1.60	1.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	293	D4N	C11-S14	-10.37	1.60	1.76
3	B	293	D4N	C11-S14	-10.15	1.60	1.76
2	D	4	NAP	O7N-C7N	7.36	1.41	1.24
2	C	3	NAP	O7N-C7N	7.34	1.41	1.24
2	A	1	NAP	O7N-C7N	7.29	1.41	1.24
2	B	2	NAP	O7N-C7N	7.18	1.41	1.24
2	B	2	NAP	C2A-N3A	3.09	1.38	1.32
2	A	1	NAP	C2A-N3A	3.06	1.38	1.32
2	D	4	NAP	C2A-N3A	3.02	1.38	1.32
2	C	3	NAP	C2A-N3A	2.99	1.38	1.32
2	B	2	NAP	C2A-N1A	2.32	1.38	1.33
2	A	1	NAP	C2A-N1A	2.28	1.38	1.33
2	C	3	NAP	C2A-N1A	2.24	1.38	1.33
2	D	4	NAP	C2A-N1A	2.21	1.38	1.33

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	4	NAP	N3A-C2A-N1A	-10.36	120.05	128.71
2	A	1	NAP	N3A-C2A-N1A	-10.18	120.20	128.71
2	B	2	NAP	N3A-C2A-N1A	-10.10	120.26	128.71
2	C	3	NAP	N3A-C2A-N1A	-9.69	120.61	128.71
3	A	293	D4N	C19-C18-N17	8.09	116.28	109.09
3	D	293	D4N	C19-C18-N17	7.43	115.69	109.09
3	C	293	D4N	C19-C18-N17	6.85	115.17	109.09
3	B	293	D4N	C19-C18-N17	6.62	114.97	109.09
3	A	293	D4N	O16-S14-O15	-6.40	107.95	119.38
3	B	293	D4N	O16-S14-O15	-6.34	108.07	119.38
3	C	293	D4N	O16-S14-O15	-6.18	108.35	119.38
3	A	293	D4N	C21-C22-N17	5.96	115.74	108.74
2	C	3	NAP	O4D-C1D-N1N	5.68	113.76	107.95
3	D	293	D4N	O16-S14-O15	-5.62	109.35	119.38
3	C	293	D4N	C21-C22-N17	5.60	115.32	108.74
2	B	2	NAP	C2D-C1D-N1N	-5.26	104.96	113.86
2	B	2	NAP	O4B-C1B-N9A	5.08	113.16	108.44
3	B	293	D4N	C21-C22-N17	5.07	114.69	108.74
2	B	2	NAP	O4D-C1D-N1N	4.69	112.75	107.95
3	D	293	D4N	C21-C22-N17	4.53	114.06	108.74
2	D	4	NAP	O4D-C1D-N1N	4.12	112.16	107.95
2	C	3	NAP	N3A-C4A-N9A	3.97	132.60	125.43
3	A	293	D4N	C6-C1-C3	-3.95	111.50	115.24
3	A	293	D4N	F4-C2-C5	-3.81	107.64	112.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	293	D4N	C22-N17-S14	-3.80	110.64	120.75
2	A	1	NAP	O4D-C1D-N1N	3.73	111.77	107.95
2	B	2	NAP	N3A-C4A-N9A	3.59	131.92	125.43
2	D	4	NAP	C2D-C1D-N1N	-3.55	107.84	113.86
3	D	293	D4N	C11-S14-N17	3.47	113.25	107.44
3	C	293	D4N	C11-S14-N17	3.47	113.25	107.44
3	A	293	D4N	C22-N17-S14	-3.39	111.72	120.75
3	A	293	D4N	C19-N20-C21	-3.35	104.33	109.85
3	B	293	D4N	F3-C2-C5	-3.35	108.23	112.49
2	D	4	NAP	N3A-C4A-N9A	3.33	131.44	125.43
2	C	3	NAP	O4B-C1B-N9A	3.32	111.53	108.44
3	B	293	D4N	C11-S14-N17	3.19	112.78	107.44
3	B	293	D4N	C22-N17-S14	-3.19	112.27	120.75
3	B	293	D4N	C1-C23-N20	-3.16	111.13	115.05
3	A	293	D4N	O1-C3-C1	-3.11	117.84	120.98
2	D	4	NAP	O4B-C1B-N9A	3.06	111.29	108.44
3	C	293	D4N	F1-C2-C5	-2.97	108.71	112.49
2	A	1	NAP	O4B-C1B-N9A	2.96	111.19	108.44
2	A	1	NAP	N3A-C4A-N9A	2.91	130.69	125.43
3	D	293	D4N	F3-C2-C5	-2.84	108.87	112.49
3	A	293	D4N	F3-C2-C5	-2.83	108.88	112.49
3	A	293	D4N	C68-C22-N17	-2.72	107.47	112.00
3	D	293	D4N	F4-C2-C5	-2.71	109.04	112.49
3	B	293	D4N	F4-C2-C5	-2.69	109.07	112.49
2	C	3	NAP	C2D-C1D-N1N	-2.65	109.36	113.86
2	B	2	NAP	C3N-C7N-N7N	2.61	120.74	117.77
3	C	293	D4N	C22-N17-S14	-2.56	113.94	120.75
2	A	1	NAP	C2D-C1D-N1N	-2.56	109.52	113.86
3	A	293	D4N	C11-S14-N17	2.56	111.72	107.44
3	C	293	D4N	C1-C23-N20	-2.55	111.89	115.05
3	D	293	D4N	C1-C23-N20	-2.55	111.89	115.05
2	C	3	NAP	C5A-C4A-N3A	-2.54	120.17	125.70
3	B	293	D4N	C19-N20-C21	-2.53	105.68	109.85
3	D	293	D4N	C14-C1-C3	-2.47	112.90	115.24
2	A	1	NAP	C1B-N9A-C4A	-2.46	122.38	126.64
3	A	293	D4N	C1-C23-N20	-2.43	112.04	115.05
2	B	2	NAP	C5A-C4A-N3A	-2.38	120.52	125.70
2	B	2	NAP	C4A-C5A-N7A	-2.34	107.52	109.52
3	C	293	D4N	F4-C2-C5	-2.32	109.53	112.49
2	A	1	NAP	N7A-C8A-N9A	-2.25	108.01	114.36
2	C	3	NAP	C4A-C5A-N7A	-2.24	107.60	109.52
2	C	3	NAP	C2A-N3A-C4A	2.22	120.32	114.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	293	D4N	C18-N17-S14	-2.21	111.82	118.25
2	B	2	NAP	C2A-N3A-C4A	2.21	120.30	114.01
2	D	4	NAP	N7A-C8A-N9A	-2.16	108.25	114.36
2	B	2	NAP	N7A-C8A-N9A	-2.16	108.25	114.36
3	A	293	D4N	C18-N17-S14	-2.14	112.02	118.25
3	C	293	D4N	O6-C5-C2	2.14	108.98	106.34
3	C	293	D4N	C21-N20-C23	-2.13	108.20	112.15
2	D	4	NAP	C4A-C5A-N7A	-2.12	107.70	109.52
2	D	4	NAP	C5A-C4A-N3A	-2.12	121.08	125.70
2	C	3	NAP	N7A-C8A-N9A	-2.12	108.37	114.36
2	D	4	NAP	C2A-N3A-C4A	2.08	119.92	114.01
3	D	293	D4N	C68-C22-N17	-2.07	108.55	112.00
3	D	293	D4N	C9-C8-C5	-2.07	119.14	121.53
3	B	293	D4N	C18-N17-S14	-2.05	112.28	118.25
2	A	1	NAP	C2N-C3N-C4N	2.05	120.63	118.31
2	A	1	NAP	C4A-C5A-N7A	-2.03	107.78	109.52
3	C	293	D4N	C14-C1-C3	-2.01	113.34	115.24

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	261/286 (91%)	0.10	6 (2%) 57 60	13, 25, 46, 54	0
1	B	265/286 (92%)	0.07	8 (3%) 48 50	13, 26, 45, 57	0
1	C	260/286 (90%)	-0.12	2 (0%) 83 84	13, 21, 37, 51	0
1	D	261/286 (91%)	0.12	8 (3%) 47 48	14, 28, 43, 50	0
All	All	1047/1144 (91%)	0.04	24 (2%) 57 60	13, 25, 44, 57	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	230	ILE	5.1
1	A	282	THR	4.1
1	A	280	TYR	3.3
1	D	230	ILE	2.9
1	A	231	VAL	2.8
1	A	23	LEU	2.8
1	D	23	LEU	2.7
1	B	228	SER	2.6
1	B	230	ILE	2.6
1	C	263	TRP	2.5
1	D	263	TRP	2.5
1	D	20	GLN	2.4
1	B	130	HIS	2.4
1	B	32	LEU	2.4
1	C	21	GLN	2.4
1	B	284	TYR	2.3
1	B	131	ASP	2.3
1	D	24	ASN	2.2
1	D	280	TYR	2.2
1	A	205	ARG	2.2
1	D	278	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	229	GLY	2.1
1	B	179[A]	MET	2.1
1	D	21	GLN	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
3	D4N	B	293	30/30	0.17	0.06	27,29,30,31	0
3	D4N	D	293	30/30	0.14	-0.24	24,25,26,27	0
3	D4N	C	293	30/30	0.12	-0.37	23,24,25,25	0
3	D4N	A	293	30/30	0.15	-0.46	24,25,30,30	0
2	NAP	C	3	48/48	0.11	-0.93	11,13,18,18	0
2	NAP	D	4	48/48	0.11	-1.02	20,22,24,25	0
2	NAP	A	1	48/48	0.11	-1.14	13,17,18,19	0
2	NAP	B	2	48/48	0.10	-1.48	15,17,22,22	0

6.5 Other polymers ⓘ

There are no such residues in this entry.