



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:40 AM GMT

PDB ID : 2BD0  
Title : Chlorobium tepidum Sepiapterin Reductase complexed with NADP and Sepiapterin  
Authors : Supangat, S.; Seo, K.H.; Choi, Y.K.; Park, Y.S.; Lee, K.H.  
Deposited on : 2005-10-19  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

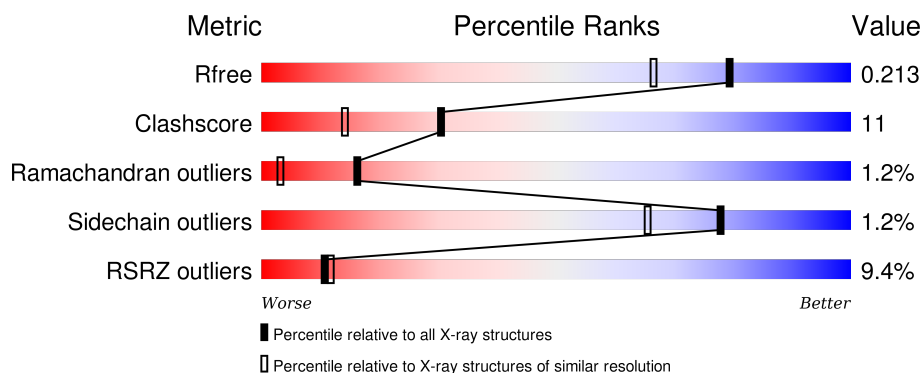
# 1 Overall quality at a glance

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))
$R_{free}$	91344	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	244	<div> <div>10%</div> <div>79%</div> <div>18%</div> <div>..</div> </div>
1	B	244	<div> <div>11%</div> <div>78%</div> <div>18%</div> <div>..</div> </div>
1	C	244	<div> <div>7%</div> <div>77%</div> <div>20%</div> <div>..</div> </div>
1	D	244	<div> <div>9%</div> <div>79%</div> <div>19%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BIO	D	900	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7974 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 sepiapterin reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	240	Total	C	N	O	S	0	0	0
			1849	1167	327	341	14			
1	B	240	Total	C	N	O	S	0	0	0
			1849	1167	327	341	14			
1	C	240	Total	C	N	O	S	0	0	0
			1849	1167	327	341	14			
1	D	240	Total	C	N	O	S	0	0	0
			1849	1167	327	341	14			

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



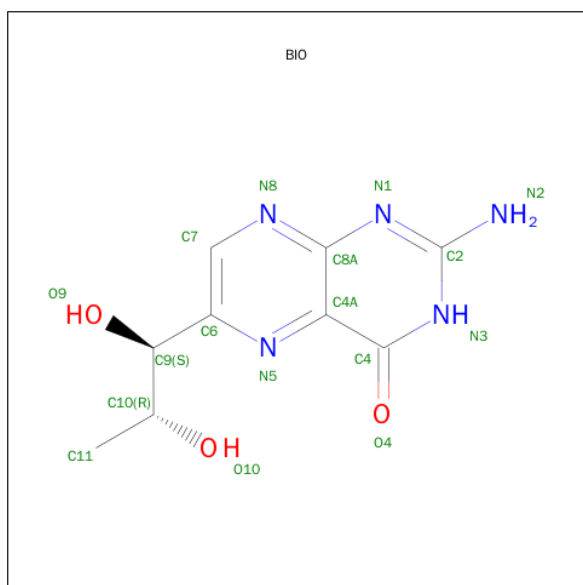
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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 BIOPTERIN (three-letter code: BIO) (formula:  $C_9H_{11}N_5O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	C	N	O	0	0
			17	9	5	3		

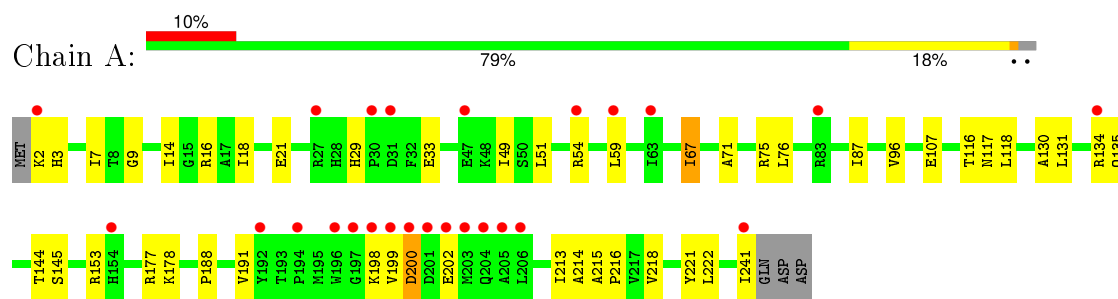
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	78	Total	O	0	0
			78	78		
4	B	74	Total	O	0	0
			74	74		
4	C	114	Total	O	0	0
			114	114		
4	D	103	Total	O	0	0
			103	103		

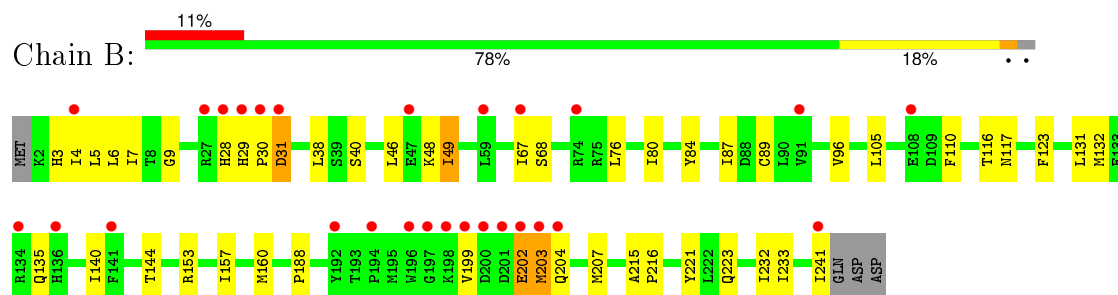
### 3 Residue-property plots [i](#)

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.

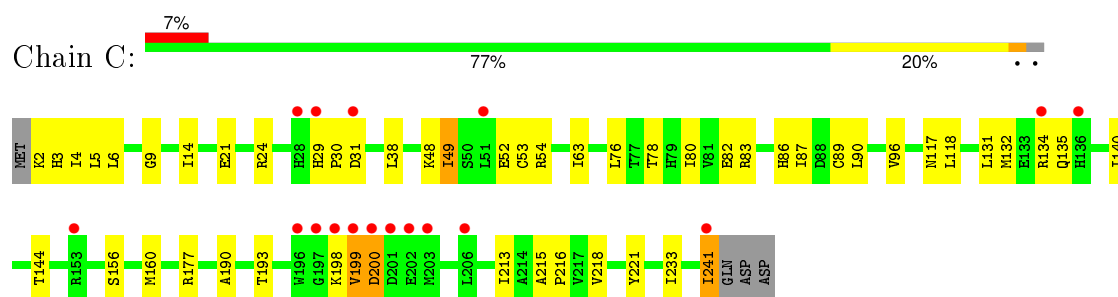
- Molecule 1: sepiapterin reductase



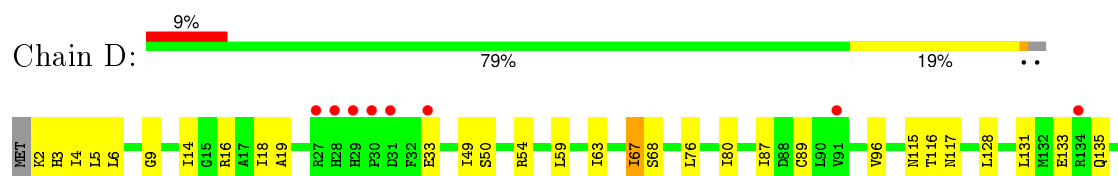
- Molecule 1: sepiapterin reductase

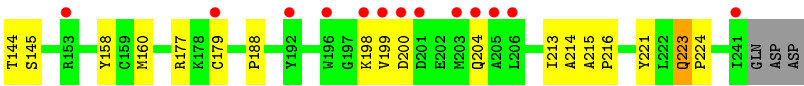


- Molecule 1: sepiapterin reductase



- Molecule 1: sepiapterin reductase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.36 Å 97.48 Å 123.24 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.90 – 1.70 31.89 – 1.69	Depositor EDS
% Data completeness (in resolution range)	99.8 (31.90-1.70) 99.0 (31.89-1.69)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.16 (at 1.69 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.200 , 0.213 0.200 , 0.213	Depositor DCC
$R_{free}$ test set	5630 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.9	Xtriage
Anisotropy	0.461	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 48.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 112538 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7974	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.91% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.32	0/1883	0.59	0/2549
1	B	0.30	0/1883	0.58	0/2549
1	C	0.33	1/1883 (0.1%)	0.62	0/2549
1	D	0.32	0/1883	0.60	0/2549
All	All	0.32	1/7532 (0.0%)	0.60	0/10196

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	134	ARG	CG-CD	5.17	1.64	1.51

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1849	0	1841	38	0
1	B	1849	0	1841	49	0
1	C	1849	0	1841	46	0
1	D	1849	0	1841	39	0
2	A	48	0	25	6	0
2	B	48	0	25	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	48	0	25	2	0
2	D	48	0	25	6	0
3	D	17	0	11	2	0
4	A	78	0	0	1	0
4	B	74	0	0	1	0
4	C	114	0	0	4	0
4	D	103	0	0	1	0
All	All	7974	0	7475	166	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:LYS:HD2	1:B:153:ARG:HH21	1.27	0.98
1:B:67:ILE:HD11	1:B:116:THR:HG23	1.49	0.95
1:D:14:ILE:O	1:D:18:ILE:HD13	1.70	0.92
1:B:5:LEU:HD22	1:B:89:CYS:HB3	1.54	0.89
1:A:14:ILE:O	1:A:18:ILE:HD13	1.74	0.88
1:B:96:VAL:H	1:B:117:ASN:HD21	1.22	0.85
1:A:14:ILE:HD11	1:A:191:VAL:HG11	1.59	0.83
1:A:87:ILE:H	1:A:135:GLN:HE22	1.26	0.83
1:D:96:VAL:H	1:D:117:ASN:HD21	1.26	0.83
1:A:96:VAL:H	1:A:117:ASN:HD21	1.26	0.82
1:B:4:ILE:HD13	1:B:84:TYR:HB3	1.61	0.82
1:A:67:ILE:HD13	2:A:800:NAP:N1A	1.94	0.82
1:C:177:ARG:HG3	4:C:2914:HOH:O	1.80	0.81
1:C:96:VAL:H	1:C:117:ASN:HD21	1.27	0.81
1:B:87:ILE:H	1:B:135:GLN:HE22	1.27	0.80
1:D:67:ILE:HD13	2:D:3800:NAP:N1A	1.98	0.79
1:D:6:LEU:HD22	1:D:80:ILE:HD11	1.64	0.79
1:C:131:LEU:O	1:C:135:GLN:HG3	1.84	0.78
1:A:215:ALA:HB3	1:A:216:PRO:HD3	1.66	0.78
1:B:132:MET:SD	1:B:140:ILE:HD11	2.24	0.77
1:A:177:ARG:HG3	4:A:853:HOH:O	1.84	0.76
1:D:87:ILE:H	1:D:135:GLN:HE22	1.31	0.76
1:D:215:ALA:HB3	1:D:216:PRO:HD3	1.68	0.76
1:B:38:LEU:HD13	1:B:49:ILE:HD12	1.67	0.74
1:C:215:ALA:HB3	1:C:216:PRO:HD3	1.69	0.74
1:A:67:ILE:HD13	2:A:800:NAP:C6A	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:LEU:HD22	1:C:80:ILE:HD11	1.73	0.70
1:D:67:ILE:HD13	2:D:3800:NAP:C6A	2.21	0.70
1:D:19:ALA:HB3	1:D:49:ILE:HD11	1.72	0.70
1:C:241:ILE:H	1:C:241:ILE:HD13	1.59	0.68
1:A:178:LYS:HD2	1:B:153:ARG:NH2	2.07	0.68
1:D:18:ILE:HD12	1:D:214:ALA:HB2	1.74	0.68
1:C:87:ILE:H	1:C:135:GLN:HE22	1.41	0.68
1:C:14:ILE:CD1	1:C:193:THR:HG21	2.24	0.67
1:C:90:LEU:HB3	1:C:140:ILE:CD1	2.24	0.67
1:A:18:ILE:HD12	1:A:214:ALA:HB2	1.75	0.67
1:B:140:ILE:N	1:B:140:ILE:HD12	2.08	0.67
1:C:5:LEU:HD22	1:C:89:CYS:HB3	1.76	0.66
1:C:14:ILE:HD12	1:C:193:THR:HG21	1.77	0.66
1:A:131:LEU:O	1:A:135:GLN:HG3	1.96	0.66
1:D:2:LYS:HD3	1:D:33:GLU:HG2	1.78	0.65
1:C:49:ILE:HD13	1:C:49:ILE:O	1.97	0.65
1:B:203:MET:O	1:B:207:MET:HG3	1.96	0.64
1:B:7:ILE:N	1:B:7:ILE:HD12	2.14	0.62
1:B:131:LEU:O	1:B:135:GLN:HG3	1.98	0.62
1:C:90:LEU:HB3	1:C:140:ILE:HD13	1.80	0.62
1:B:30:PRO:O	1:B:31:ASP:HB3	2.00	0.61
1:B:144:THR:O	2:B:1800:NAP:H6N	2.00	0.61
1:C:63:ILE:HD13	1:C:76:LEU:HD23	1.82	0.61
1:D:50:SER:OG	1:D:54:ARG:NH1	2.35	0.59
3:D:900:BIO:H10	4:D:3903:HOH:O	2.03	0.58
1:C:14:ILE:H	1:C:14:ILE:HD12	1.66	0.58
1:C:90:LEU:HD23	1:C:140:ILE:HD12	1.86	0.57
1:B:48:LYS:NZ	1:B:48:LYS:HB2	2.18	0.57
1:A:9:GLY:HA2	2:A:800:NAP:H1B	1.87	0.56
1:A:213:ILE:O	1:A:216:PRO:HD2	2.05	0.56
1:D:9:GLY:HA2	2:D:3800:NAP:H1B	1.87	0.55
1:B:3:HIS:HD2	1:B:221:TYR:OH	1.88	0.55
1:C:241:ILE:H	1:C:241:ILE:CD1	2.20	0.55
1:D:158:TYR:HE2	3:D:900:BIO:HO9	1.54	0.55
1:C:83:ARG:HH11	1:C:83:ARG:HG2	1.71	0.54
1:C:38:LEU:HD13	1:C:49:ILE:HD12	1.87	0.54
1:B:9:GLY:HA2	2:B:1800:NAP:H1B	1.90	0.54
1:B:67:ILE:HD12	1:B:67:ILE:C	2.26	0.54
1:D:188:PRO:HG2	2:D:3800:NAP:C5N	2.37	0.54
1:C:14:ILE:N	1:C:14:ILE:HD12	2.22	0.54
1:B:76:LEU:O	1:B:80:ILE:HD13	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:ASP:O	1:A:202:GLU:N	2.41	0.54
1:A:7:ILE:HD12	1:A:7:ILE:N	2.23	0.54
1:C:2:LYS:N	4:C:2904:HOH:O	2.40	0.53
1:C:78:THR:HB	1:C:82:GLU:OE2	2.07	0.53
1:D:5:LEU:HG	1:D:89:CYS:HB3	1.90	0.53
1:C:30:PRO:HB3	4:C:2910:HOH:O	2.07	0.53
1:B:233:ILE:N	1:B:233:ILE:HD12	2.24	0.53
1:A:153:ARG:HH11	1:A:153:ARG:HG3	1.73	0.53
1:D:3:HIS:HD2	1:D:221:TYR:OH	1.91	0.53
1:A:144:THR:O	2:A:800:NAP:H6N	2.08	0.53
1:C:199:VAL:O	1:C:200:ASP:CB	2.57	0.53
1:C:3:HIS:HD2	1:C:221:TYR:OH	1.92	0.52
1:B:188:PRO:HG2	2:B:1800:NAP:C5N	2.39	0.52
1:A:188:PRO:HG2	2:A:800:NAP:C5N	2.38	0.52
1:B:40:SER:HB3	1:B:46:LEU:HD21	1.91	0.52
1:D:67:ILE:HD11	1:D:116:THR:HG23	1.92	0.52
1:B:28:HIS:C	1:B:30:PRO:HD3	2.30	0.52
1:D:223:GLN:HE21	1:D:224:PRO:HD2	1.73	0.52
1:B:49:ILE:O	1:B:49:ILE:HD13	2.10	0.51
1:D:2:LYS:HZ1	1:D:59:LEU:HD11	1.75	0.51
1:C:29:HIS:NE2	1:C:31:ASP:HB2	2.24	0.51
1:D:63:ILE:HD13	1:D:76:LEU:HD23	1.91	0.51
1:A:3:HIS:HD2	1:A:221:TYR:OH	1.93	0.51
1:C:9:GLY:HA2	2:C:2800:NAP:H1B	1.90	0.51
1:D:144:THR:O	2:D:3800:NAP:H6N	2.11	0.51
1:D:2:LYS:HZ3	1:D:33:GLU:CD	2.13	0.51
1:C:144:THR:O	2:C:2800:NAP:H6N	2.09	0.51
1:A:16:ARG:HG3	1:A:49:ILE:HD13	1.92	0.51
1:D:18:ILE:HD12	1:D:214:ALA:CB	2.40	0.51
1:C:86:HIS:HB2	1:C:135:GLN:NE2	2.26	0.50
1:D:200:ASP:O	1:D:204:GLN:HG3	2.12	0.50
1:B:30:PRO:O	1:B:31:ASP:CB	2.60	0.50
1:B:6:LEU:C	1:B:7:ILE:HD12	2.33	0.49
1:D:16:ARG:HG3	1:D:49:ILE:HD12	1.94	0.49
1:C:241:ILE:N	1:C:241:ILE:HD13	2.27	0.49
1:A:241:ILE:HD12	1:A:241:ILE:C	2.32	0.49
1:A:18:ILE:HD12	1:A:214:ALA:CB	2.40	0.49
1:C:54:ARG:HH11	1:C:54:ARG:HG2	1.78	0.49
1:A:67:ILE:HD11	1:A:116:THR:HG23	1.94	0.49
1:D:213:ILE:O	1:D:216:PRO:HD2	2.13	0.49
1:C:233:ILE:HD12	1:C:233:ILE:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:80:ILE:HD12	1:D:128:LEU:HD21	1.94	0.48
1:A:2:LYS:NZ	1:A:33:GLU:HG2	2.28	0.47
1:A:2:LYS:NZ	1:A:59:LEU:HD11	2.29	0.47
1:B:49:ILE:C	1:B:49:ILE:HD13	2.34	0.47
1:A:118:LEU:HD22	1:B:160:MET:CE	2.43	0.47
1:B:241:ILE:HG23	4:B:1838:HOH:O	2.14	0.47
1:C:190:ALA:HB2	1:C:241:ILE:HD12	1.98	0.47
1:B:199:VAL:CB	1:B:204:GLN:HG3	2.45	0.47
1:B:105:LEU:HD13	1:B:157:ILE:HG12	1.97	0.47
1:C:118:LEU:HD22	1:D:160:MET:HE2	1.97	0.46
1:B:5:LEU:HD22	1:B:89:CYS:CB	2.34	0.46
1:B:67:ILE:HD12	1:B:68:SER:N	2.30	0.46
1:B:202:GLU:O	1:B:204:GLN:N	2.49	0.46
1:B:29:HIS:ND1	1:B:31:ASP:OD1	2.45	0.45
1:B:67:ILE:CD1	1:B:116:THR:HA	2.45	0.45
1:C:4:ILE:HG12	1:C:86:HIS:CE1	2.52	0.45
1:A:21:GLU:HG3	1:A:218:VAL:HG21	1.99	0.45
1:B:202:GLU:O	1:B:203:MET:C	2.55	0.45
1:C:49:ILE:C	1:C:49:ILE:HD13	2.37	0.45
1:A:71:ALA:O	1:A:75:ARG:HG3	2.17	0.45
1:D:131:LEU:O	1:D:135:GLN:HG3	2.17	0.45
1:A:130:ALA:O	1:A:134:ARG:HG3	2.18	0.44
1:B:110:PHE:HD2	1:B:157:ILE:HD12	1.83	0.44
1:A:153:ARG:NH1	1:A:153:ARG:HG3	2.32	0.43
1:A:51:LEU:HD23	1:A:54:ARG:NH2	2.33	0.43
1:D:117:ASN:HD22	1:D:117:ASN:N	2.16	0.43
1:B:117:ASN:N	1:B:117:ASN:HD22	2.15	0.43
1:D:67:ILE:CD1	2:D:3800:NAP:C6A	2.95	0.43
1:A:67:ILE:CD1	2:A:800:NAP:C6A	2.93	0.43
1:C:213:ILE:O	1:C:216:PRO:HD2	2.19	0.43
1:D:16:ARG:HA	1:D:49:ILE:HD12	2.00	0.43
1:D:63:ILE:O	1:D:63:ILE:HG23	2.18	0.42
1:D:68:SER:HB2	1:D:115:ASN:HB3	1.99	0.42
1:A:144:THR:O	1:A:145:SER:HB2	2.19	0.42
1:C:54:ARG:NH1	1:C:54:ARG:HG2	2.34	0.42
1:D:133:GLU:HG3	1:D:179:CYS:SG	2.59	0.42
1:A:29:HIS:NE2	1:A:222:LEU:HD13	2.34	0.42
1:B:67:ILE:HG13	2:B:1800:NAP:N1A	2.35	0.42
1:C:90:LEU:HB3	1:C:140:ILE:HD12	1.98	0.42
1:B:232:ILE:C	1:B:233:ILE:HD12	2.40	0.42
1:C:156:SER:O	1:C:160:MET:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:ARG:NH1	4:C:2907:HOH:O	2.52	0.42
1:D:4:ILE:O	1:D:87:ILE:HD12	2.19	0.42
1:A:117:ASN:HD22	1:A:117:ASN:N	2.17	0.41
1:B:215:ALA:HB3	1:B:216:PRO:CD	2.51	0.41
1:B:67:ILE:HD11	1:B:116:THR:CG2	2.34	0.41
1:D:144:THR:O	1:D:145:SER:HB2	2.20	0.41
1:C:21:GLU:HG3	1:C:218:VAL:HG21	2.02	0.41
1:D:5:LEU:N	1:D:5:LEU:HD12	2.35	0.41
1:B:7:ILE:CD1	1:B:7:ILE:N	2.83	0.41
1:A:107:GLU:HA	1:B:123:PHE:CZ	2.56	0.41
1:C:48:LYS:O	1:C:52:GLU:HG3	2.21	0.41
1:B:48:LYS:HZ2	1:B:48:LYS:HB2	1.84	0.41
1:C:118:LEU:HD22	1:D:160:MET:CE	2.52	0.40
1:B:132:MET:SD	1:B:140:ILE:CD1	3.04	0.40
1:C:132:MET:SD	1:C:140:ILE:HD11	2.61	0.40
1:C:49:ILE:CD1	1:C:53:CYS:SG	3.10	0.40
1:A:118:LEU:HD22	1:B:160:MET:HE2	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	238/244 (98%)	227 (95%)	8 (3%)	3 (1%)	15	2
1	B	238/244 (98%)	225 (94%)	10 (4%)	3 (1%)	15	2
1	C	238/244 (98%)	227 (95%)	8 (3%)	3 (1%)	15	2
1	D	238/244 (98%)	232 (98%)	4 (2%)	2 (1%)	24	7
All	All	952/976 (98%)	911 (96%)	30 (3%)	11 (1%)	16	3

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	199	VAL
1	A	200	ASP
1	B	31	ASP
1	B	202	GLU
1	C	198	LYS
1	C	199	VAL
1	D	198	LYS
1	A	198	LYS
1	B	203	MET
1	C	200	ASP
1	D	199	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	194/203 (96%)	192 (99%)	2 (1%)	82	72
1	B	194/203 (96%)	192 (99%)	2 (1%)	82	72
1	C	194/203 (96%)	192 (99%)	2 (1%)	82	72
1	D	194/203 (96%)	191 (98%)	3 (2%)	72	56
All	All	776/812 (96%)	767 (99%)	9 (1%)	78	65

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ILE
1	A	76	LEU
1	B	49	ILE
1	B	223	GLN
1	C	49	ILE
1	C	241	ILE
1	D	67	ILE
1	D	177	ARG
1	D	223	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	115	ASN
1	A	117	ASN
1	A	135	GLN
1	A	180	ASN
1	A	204	GLN
1	B	3	HIS
1	B	115	ASN
1	B	117	ASN
1	B	135	GLN
1	B	223	GLN
1	C	3	HIS
1	C	115	ASN
1	C	117	ASN
1	C	135	GLN
1	C	180	ASN
1	D	3	HIS
1	D	115	ASN
1	D	117	ASN
1	D	135	GLN
1	D	180	ASN
1	D	204	GLN
1	D	223	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

5 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	800	-	42,52,52	1.07	3 (7%)	54,80,80	1.79	7 (12%)
2	NAP	B	1800	-	42,52,52	1.07	3 (7%)	54,80,80	1.79	7 (12%)
2	NAP	C	2800	-	42,52,52	1.06	3 (7%)	54,80,80	1.75	4 (7%)
2	NAP	D	3800	-	42,52,52	1.07	3 (7%)	54,80,80	1.77	6 (11%)
3	BIO	D	900	-	16,18,18	1.83	4 (25%)	13,26,26	2.97	8 (61%)

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	800	-	-	0/27/67/67	0/5/5/5
2	NAP	B	1800	-	-	0/27/67/67	0/5/5/5
2	NAP	C	2800	-	-	0/27/67/67	0/5/5/5
2	NAP	D	3800	-	-	0/27/67/67	0/5/5/5
3	BIO	D	900	-	-	0/8/8/8	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	900	BIO	C7-N8	2.20	1.35	1.31
2	C	2800	NAP	O4B-C1B	2.20	1.44	1.41
2	B	1800	NAP	O4B-C1B	2.24	1.44	1.41
2	D	3800	NAP	O4B-C1B	2.31	1.44	1.41
2	A	800	NAP	O4B-C1B	2.32	1.44	1.41
2	A	800	NAP	O4D-C1D	2.37	1.44	1.41
2	D	3800	NAP	O4D-C1D	2.37	1.44	1.41
2	C	2800	NAP	O4D-C1D	2.38	1.44	1.41
2	B	1800	NAP	O4D-C1D	2.39	1.44	1.41
3	D	900	BIO	C4-N3	2.72	1.38	1.33
2	C	2800	NAP	P2B-O1X	3.09	1.61	1.51
2	D	3800	NAP	P2B-O1X	3.10	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	800	NAP	P2B-O1X	3.10	1.61	1.51
2	B	1800	NAP	P2B-O1X	3.12	1.61	1.51
3	D	900	BIO	C6-N5	3.31	1.35	1.32
3	D	900	BIO	C4-C4A	4.10	1.49	1.41

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3800	NAP	N3A-C2A-N1A	-10.41	120.92	128.89
2	A	800	NAP	N3A-C2A-N1A	-10.24	121.05	128.89
2	B	1800	NAP	N3A-C2A-N1A	-10.23	121.06	128.89
2	C	2800	NAP	N3A-C2A-N1A	-10.21	121.08	128.89
3	D	900	BIO	C4A-C4-N3	-4.29	117.72	123.59
3	D	900	BIO	C4-C4A-C8A	-3.93	117.42	119.94
3	D	900	BIO	N1-C2-N3	-3.32	122.38	127.44
2	B	1800	NAP	PN-O3-PA	-3.20	123.75	132.73
2	A	800	NAP	PN-O3-PA	-2.90	124.60	132.73
3	D	900	BIO	C7-C6-N5	-2.83	119.27	121.42
2	D	3800	NAP	PN-O3-PA	-2.82	124.81	132.73
2	C	2800	NAP	PN-O3-PA	-2.72	125.08	132.73
2	B	1800	NAP	C3B-C2B-C1B	-2.32	98.23	102.73
2	B	1800	NAP	C3N-C7N-N7N	-2.22	115.39	117.82
2	A	800	NAP	C3N-C7N-N7N	-2.21	115.40	117.82
2	D	3800	NAP	C4A-C5A-N7A	-2.05	107.59	109.48
2	A	800	NAP	C4A-C5A-N7A	-2.04	107.60	109.48
2	B	1800	NAP	C4B-O4B-C1B	-2.04	107.47	109.72
2	C	2800	NAP	C4A-C5A-N7A	-2.03	107.61	109.48
2	D	3800	NAP	C3B-C2B-C1B	-2.02	98.82	102.73
2	A	800	NAP	C4B-O4B-C1B	-2.02	107.50	109.72
2	A	800	NAP	C3B-C2B-C1B	-2.01	98.83	102.73
2	D	3800	NAP	C3N-C7N-N7N	-2.01	115.61	117.82
2	B	1800	NAP	C4A-C5A-N7A	-2.01	107.63	109.48
2	C	2800	NAP	O4D-C1D-N1N	2.72	111.12	108.13
2	D	3800	NAP	O4D-C1D-N1N	2.79	111.20	108.13
2	B	1800	NAP	O4D-C1D-N1N	3.27	111.72	108.13
3	D	900	BIO	C4-C4A-N5	3.44	122.90	118.72
3	D	900	BIO	C7-N8-C8A	3.48	121.03	116.93
2	A	800	NAP	O4D-C1D-N1N	3.56	112.04	108.13
3	D	900	BIO	C4-N3-C2	3.68	121.04	115.94
3	D	900	BIO	N8-C8A-N1	4.14	122.07	116.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	800	NAP	6	0
2	B	1800	NAP	4	0
2	C	2800	NAP	2	0
2	D	3800	NAP	6	0
3	D	900	BIO	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	240/244 (98%)	0.53	25 (10%) 8 9	14, 21, 46, 60	0
1	B	240/244 (98%)	0.68	27 (11%) 7 7	14, 23, 49, 68	0
1	C	240/244 (98%)	0.36	17 (7%) 19 21	13, 19, 39, 55	0
1	D	240/244 (98%)	0.46	21 (8%) 12 13	14, 20, 41, 57	0
All	All	960/976 (98%)	0.51	90 (9%) 11 12	13, 21, 41, 68	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	199	VAL	9.5
1	D	28	HIS	8.0
1	B	30	PRO	7.9
1	C	199	VAL	7.9
1	D	241	ILE	7.8
1	C	241	ILE	7.4
1	B	199	VAL	6.8
1	D	30	PRO	6.8
1	B	201	ASP	6.5
1	B	203	MET	6.4
1	C	51	LEU	5.9
1	D	199	VAL	5.7
1	D	206	LEU	5.7
1	A	30	PRO	5.4
1	D	29	HIS	5.4
1	B	198	LYS	5.4
1	A	200	ASP	5.3
1	A	241	ILE	5.1
1	A	201	ASP	5.0
1	B	28	HIS	4.9
1	B	202	GLU	4.8

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Mol	Chain	Res	Type	RSRZ
1	D	31	ASP	4.8
1	D	205	ALA	4.8
1	A	203	MET	4.7
1	B	241	ILE	4.7
1	A	198	LYS	4.6
1	D	200	ASP	4.5
1	A	206	LEU	4.3
1	A	27	ARG	4.2
1	B	134	ARG	4.2
1	A	47	GLU	4.2
1	B	31	ASP	4.2
1	C	206	LEU	4.1
1	A	196	TRP	4.1
1	D	203	MET	4.1
1	B	200	ASP	4.0
1	B	29	HIS	4.0
1	A	197	GLY	3.9
1	D	198	LYS	3.8
1	C	201	ASP	3.8
1	A	134	ARG	3.7
1	C	28	HIS	3.7
1	B	196	TRP	3.5
1	B	136	HIS	3.5
1	D	27	ARG	3.5
1	C	203	MET	3.4
1	C	200	ASP	3.4
1	C	134	ARG	3.3
1	A	192	TYR	3.2
1	A	54	ARG	3.1
1	C	29	HIS	3.0
1	D	196	TRP	3.0
1	C	31	ASP	3.0
1	A	205	ALA	3.0
1	C	196	TRP	3.0
1	D	153	ARG	2.9
1	A	204	GLN	2.9
1	B	59	LEU	2.8
1	D	33	GLU	2.8
1	D	201	ASP	2.8
1	A	31	ASP	2.7
1	D	134	ARG	2.7
1	B	4	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	194	PRO	2.7
1	A	2	LYS	2.7
1	B	47	GLU	2.6
1	A	83	ARG	2.5
1	D	204	GLN	2.5
1	C	198	LYS	2.5
1	B	108	GLU	2.4
1	A	202	GLU	2.4
1	B	192	TYR	2.3
1	B	204	GLN	2.3
1	B	197	GLY	2.3
1	B	194	PRO	2.3
1	A	59	LEU	2.3
1	C	136	HIS	2.3
1	B	74	ARG	2.2
1	B	67	ILE	2.2
1	B	91	VAL	2.2
1	D	91	VAL	2.2
1	C	197	GLY	2.2
1	C	153	ARG	2.2
1	C	202	GLU	2.2
1	A	154	HIS	2.2
1	B	27	ARG	2.1
1	D	179	CYS	2.1
1	D	192	TYR	2.1
1	B	141	PHE	2.1
1	A	63	ILE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	BIO	D	900	17/17	0.52	0.28	5.58	42,49,51,51	0
2	NAP	A	800	48/48	0.94	0.10	-0.17	19,22,26,29	0
2	NAP	B	1800	48/48	0.92	0.10	-0.29	21,25,29,29	0
2	NAP	C	2800	48/48	0.97	0.10	-0.31	15,17,20,21	0
2	NAP	D	3800	48/48	0.96	0.07	-0.99	17,19,21,23	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.