



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 10:09 PM GMT

PDB ID : 3F8R
Title : Crystal structure of Sulfolobus solfataricus Thioredoxin reductase B3 in complex with two NADP molecules
Authors : Ruggiero, A.; Masullo, M.; Ruocco, M.R.; Arcari, P.; Zagari, A.; Vitagliano, L.
Deposited on : 2008-11-13
Resolution : 1.95 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>

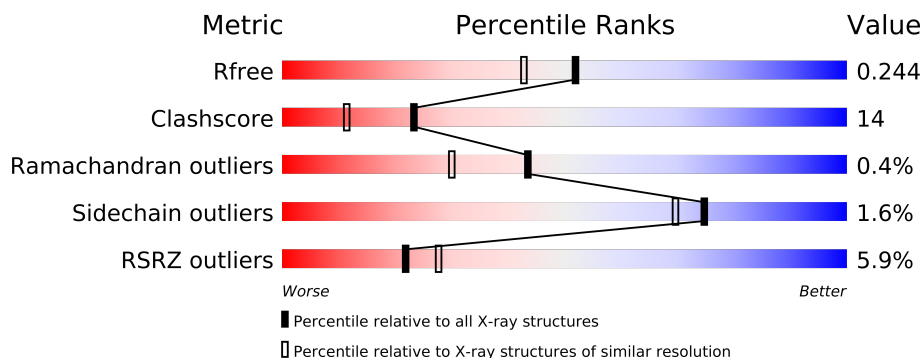
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.95 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	1321 (1.96-1.96)
Clashscore	79885	1488 (1.96-1.96)
Ramachandran outliers	78287	1475 (1.96-1.96)
Sidechain outliers	78261	1475 (1.96-1.96)
RSRZ outliers	66119	1321 (1.96-1.96)

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	323	
1	B	323	
1	C	323	
1	D	323	

2 Entry composition i

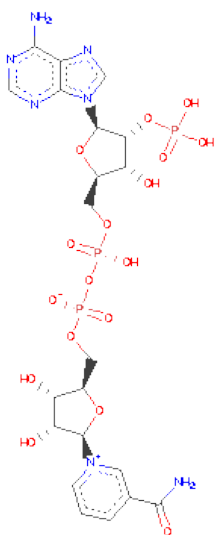
There are 3 unique types of molecules in this entry. The entry contains 10058 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Thioredoxin reductase (TrxB-3).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	0	0	0
			2367	1523	395	443	6			
1	B	309	Total	C	N	O	S	0	0	0
			2375	1527	396	446	6			
1	C	307	Total	C	N	O	S	0	0	0
			2356	1517	391	442	6			
1	D	298	Total	C	N	O	S	0	0	0
			2285	1469	381	429	6			

- 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	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

- Molecule 3 is water.

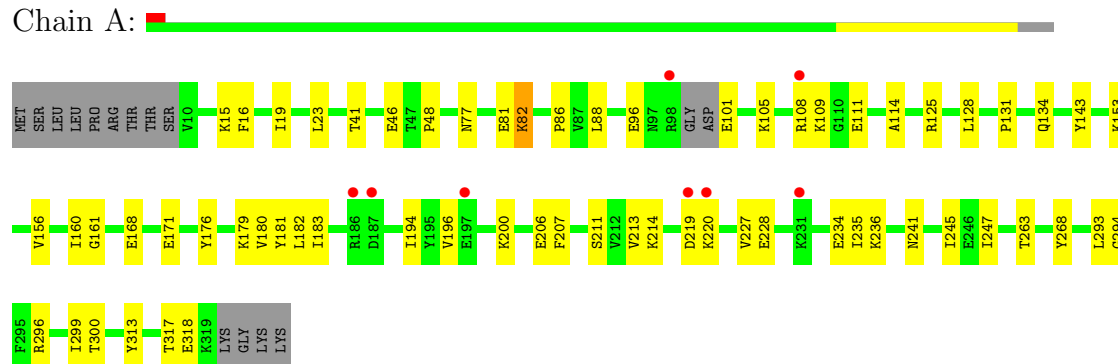
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	88	Total	O	0	0
			88	88		
3	B	82	Total	O	0	0
			82	82		
3	C	89	Total	O	0	0
			89	89		
3	D	101	Total	O	0	0
			101	101		

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.

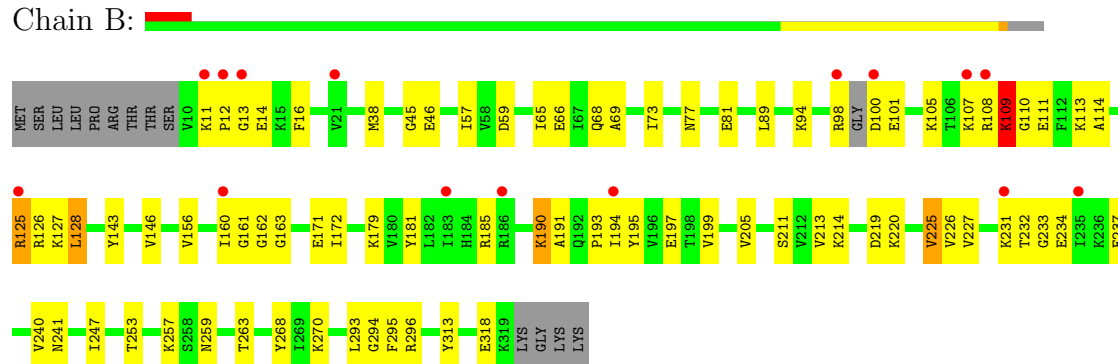
• Molecule 1: Thioredoxin reductase (TrxB-3)

Chain A:



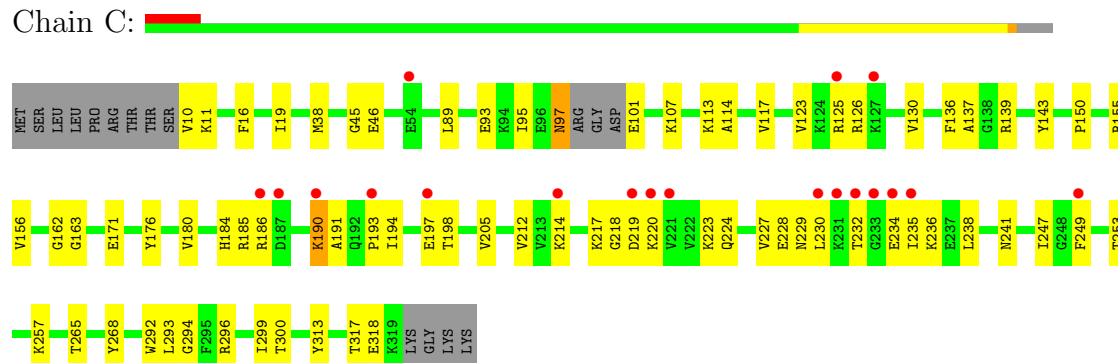
• Molecule 1: Thioredoxin reductase (TrxB-3)

Chain B:



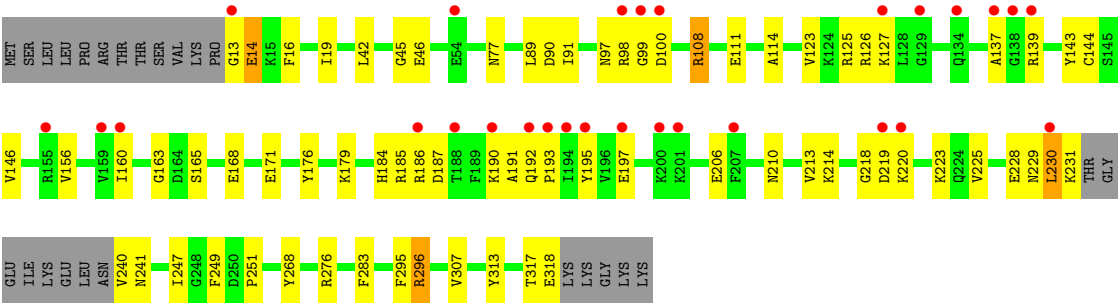
• Molecule 1: Thioredoxin reductase (TrxB-3)

Chain C:



● Molecule 1: Thioredoxin reductase (TrxB-3)

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.87Å 123.42Å 127.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 1.95 19.97 – 1.95	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-1.95) 86.2 (19.97-1.95)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 1.94Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.208 , 0.257 0.210 , 0.244	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	19.7	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 39.1	EDS
Estimated twinning fraction	0.014 for -h,l,k	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 80321 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10058	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.81% 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

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	0.54	0/2407	0.71	0/3252
1	B	0.55	0/2415	0.72	1/3263 (0.0%)
1	C	0.57	0/2396	0.71	0/3238
1	D	0.54	0/2324	0.71	0/3141
All	All	0.55	0/9542	0.71	1/12894 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	13	GLY	N-CA-C	-5.01	100.57	113.10

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	2367	0	2428	62	0
1	B	2375	0	2432	78	0
1	C	2356	0	2415	79	0
1	D	2285	0	2330	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	79	0	36	7	0
2	B	79	0	36	8	0
2	C	79	0	36	10	0
2	D	78	0	36	6	0
3	A	88	0	0	11	0
3	B	82	0	0	12	0
3	C	89	0	0	3	0
3	D	101	0	0	7	0
All	All	10058	0	9749	281	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 14.

All (281) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:156:VAL:H	1:B:241:ASN:ND2	1.61	0.97
1:A:105:LYS:HG2	1:A:111:GLU:HG2	1.52	0.90
1:C:190:LYS:H	1:C:190:LYS:HD3	1.36	0.89
1:A:219:ASP:CG	1:A:220:LYS:H	1.77	0.89
1:D:214:LYS:HD2	1:D:228:GLU:HB2	1.55	0.89
1:B:156:VAL:H	1:B:241:ASN:HD22	0.91	0.87
2:A:4001:NAP:H2D	3:A:5128:HOH:O	1.77	0.85
1:B:125:ARG:HH12	1:B:127:LYS:HB3	1.43	0.84
1:C:219:ASP:CG	1:C:220:LYS:H	1.82	0.82
1:A:179:LYS:HE2	1:A:181:TYR:CE1	2.14	0.82
1:B:156:VAL:N	1:B:241:ASN:HD22	1.74	0.82
1:A:179:LYS:HE2	1:A:181:TYR:CZ	2.14	0.81
1:B:190:LYS:HE3	2:B:4002:NAP:H4B	1.62	0.81
1:D:146:VAL:HG13	3:D:5318:HOH:O	1.82	0.80
1:A:88:LEU:HD11	1:A:109:LYS:HD3	1.64	0.80
1:B:109:LYS:HD2	1:B:109:LYS:H	1.46	0.80
1:D:214:LYS:HD2	1:D:228:GLU:CB	2.10	0.79
1:C:232:THR:HG21	1:C:234:GLU:HB2	1.64	0.78
1:B:193:PRO:O	1:B:197:GLU:HG2	1.82	0.77
1:B:195:TYR:O	1:B:199:VAL:HG23	1.84	0.77
1:C:125:ARG:HD2	1:C:143:TYR:CD1	2.21	0.75
1:A:96:GLU:OE1	1:A:105:LYS:HE3	1.87	0.74
1:C:214:LYS:HE3	1:C:228:GLU:HB2	1.68	0.74
1:B:125:ARG:HD2	1:B:143:TYR:CD1	2.21	0.74
1:B:190:LYS:CE	2:B:4002:NAP:H4B	2.17	0.74
1:B:126:ARG:NH1	3:B:5025:HOH:O	2.20	0.74
1:A:88:LEU:HD11	1:A:109:LYS:CD	2.17	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:232:THR:CG2	1:C:234:GLU:HB2	2.18	0.73
1:B:190:LYS:HD3	3:B:5090:HOH:O	1.89	0.73
1:B:162:GLY:C	1:B:190:LYS:HE2	2.10	0.72
1:C:190:LYS:CE	2:C:4003:NAP:H4B	2.19	0.72
1:A:156:VAL:H	1:A:241:ASN:HD22	1.36	0.72
1:C:313:TYR:OH	1:D:171:GLU:HG3	1.90	0.71
1:D:156:VAL:H	1:D:241:ASN:HD22	1.38	0.71
1:B:190:LYS:NZ	2:B:4002:NAP:H4B	2.05	0.71
1:B:185:ARG:HG2	3:B:5001:HOH:O	1.90	0.70
1:C:194:ILE:HG12	1:D:318:GLU:HG2	1.74	0.70
1:B:105:LYS:HG3	1:B:111:GLU:HG2	1.74	0.69
1:B:226:VAL:HG22	1:B:237:GLU:HG2	1.75	0.69
1:B:98:ARG:HB2	3:B:5210:HOH:O	1.91	0.69
1:B:163:GLY:N	1:B:190:LYS:HE2	2.08	0.68
1:A:219:ASP:CG	1:A:220:LYS:N	2.48	0.67
1:C:214:LYS:HE3	1:C:235:ILE:HD12	1.75	0.67
1:C:194:ILE:CG1	1:D:318:GLU:HG2	2.25	0.67
1:C:234:GLU:O	1:C:235:ILE:HD13	1.95	0.67
1:D:225:VAL:HG13	1:D:240:VAL:HG21	1.78	0.66
1:C:163:GLY:N	1:C:190:LYS:HE2	2.11	0.65
1:A:128:LEU:HD13	3:A:5057:HOH:O	1.94	0.65
2:B:4002:NAP:H8A	3:B:5025:HOH:O	1.97	0.65
1:A:171:GLU:HG3	1:B:313:TYR:OH	1.97	0.65
1:D:184:HIS:NE2	1:D:186:ARG:HB2	2.12	0.65
1:B:109:LYS:HD2	1:B:109:LYS:N	2.10	0.64
1:D:190:LYS:NZ	2:D:4004:NAP:H4B	2.12	0.64
1:C:185:ARG:HG2	3:C:5012:HOH:O	1.97	0.64
1:C:11:LYS:HD2	1:C:11:LYS:N	2.13	0.64
1:B:125:ARG:NH1	1:B:127:LYS:HB3	2.11	0.63
1:C:219:ASP:CG	1:C:220:LYS:N	2.51	0.63
1:B:98:ARG:HB3	1:B:101:GLU:O	1.97	0.63
1:B:125:ARG:HD2	1:B:143:TYR:CE1	2.33	0.63
1:D:160:ILE:CD1	1:D:213:VAL:HG21	2.28	0.63
1:D:168:GLU:HB2	1:D:195:TYR:HE2	1.63	0.63
1:D:90:ASP:OD1	1:D:108:ARG:HD2	1.98	0.63
1:B:125:ARG:HH22	1:B:127:LYS:HD3	1.63	0.62
1:D:268:TYR:OH	1:D:296:ARG:NH2	2.24	0.62
1:C:229:ASN:HB3	1:C:232:THR:HB	1.82	0.62
1:B:268:TYR:OH	1:B:296:ARG:NH2	2.33	0.62
1:B:294:GLY:C	3:B:5127:HOH:O	2.38	0.62
1:A:313:TYR:OH	1:B:171:GLU:HG3	2.00	0.62
1:B:190:LYS:HZ1	2:B:4002:NAP:H4B	1.64	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:82:LYS:HE2	1:B:59:ASP:OD2	1.99	0.61
1:A:105:LYS:HG2	1:A:111:GLU:CG	2.29	0.61
1:C:93:GLU:OE2	1:C:107:LYS:HG3	2.00	0.61
1:B:163:GLY:CA	1:B:190:LYS:HE2	2.30	0.61
1:B:179:LYS:HE3	1:B:181:TYR:CZ	2.36	0.61
1:C:190:LYS:HZ1	2:C:4003:NAP:H4B	1.65	0.61
1:B:101:GLU:OE1	1:B:113:LYS:HD3	2.01	0.61
1:C:190:LYS:N	1:C:190:LYS:HD3	2.13	0.61
1:A:179:LYS:NZ	1:A:206:GLU:OE1	2.22	0.61
1:A:234:GLU:OE1	1:A:236:LYS:HE3	2.00	0.61
1:A:77:ASN:HB2	3:A:5213:HOH:O	1.99	0.61
1:C:190:LYS:HE3	2:C:4003:NAP:O3B	2.00	0.60
2:B:4002:NAP:H3B	3:B:5025:HOH:O	2.00	0.60
1:C:218:GLY:HA2	1:C:223:LYS:HB2	1.83	0.60
1:C:268:TYR:OH	1:C:296:ARG:NH2	2.34	0.60
1:B:161:GLY:HA3	3:B:5045:HOH:O	2.01	0.60
1:D:125:ARG:HD2	1:D:143:TYR:CE1	2.36	0.60
1:C:190:LYS:NZ	2:C:4003:NAP:H4B	2.16	0.60
1:C:214:LYS:CE	1:C:235:ILE:HD12	2.32	0.60
1:A:168:GLU:OE2	2:A:4001:NAP:H4N	2.02	0.60
1:B:125:ARG:HH12	1:B:127:LYS:CB	2.14	0.59
1:C:318:GLU:HG3	3:C:5292:HOH:O	2.01	0.59
1:A:161:GLY:HA3	3:A:5067:HOH:O	2.02	0.59
1:C:125:ARG:HD2	1:C:143:TYR:CE1	2.37	0.59
1:B:105:LYS:CG	1:B:111:GLU:HG2	2.33	0.58
1:D:230:LEU:O	1:D:231:LYS:HG3	2.03	0.58
1:D:125:ARG:HD2	1:D:143:TYR:CZ	2.38	0.58
1:A:214:LYS:HD2	1:A:228:GLU:HB2	1.86	0.58
1:C:253:THR:HG22	1:C:257:LYS:HE3	1.85	0.58
1:A:101:GLU:N	3:A:5130:HOH:O	2.37	0.58
1:B:57:ILE:HD13	1:B:68:GLN:OE1	2.04	0.58
1:C:227:VAL:HG12	1:C:228:GLU:N	2.17	0.57
1:C:101:GLU:OE2	1:C:113:LYS:HD2	2.04	0.57
1:B:128:LEU:HD13	1:B:247:ILE:HD13	1.86	0.57
1:A:125:ARG:HD2	1:A:143:TYR:CD1	2.40	0.57
1:D:219:ASP:CG	1:D:220:LYS:H	2.07	0.57
1:B:160:ILE:CD1	1:B:213:VAL:HG21	2.34	0.57
1:A:82:LYS:NZ	1:B:66:GLU:OE2	2.32	0.56
1:A:153:LYS:HG3	3:A:5208:HOH:O	2.05	0.56
1:C:156:VAL:H	1:C:241:ASN:HD22	1.52	0.56
2:C:4003:NAP:O2N	2:C:4003:NAP:H3D	2.05	0.56
1:D:165:SER:HB2	2:D:4004:NAP:O1N	2.06	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:296:ARG:HH22	2:A:4001:NAP:H51N	1.69	0.56
1:A:15:LYS:HG3	1:A:16:PHE:N	2.20	0.56
1:C:38:MET:HG2	1:D:176:TYR:CZ	2.40	0.56
1:A:294:GLY:HA3	2:A:4001:NAP:H1D	1.87	0.56
1:B:214:LYS:HE2	1:B:214:LYS:HA	1.87	0.55
1:A:108:ARG:NH1	1:A:109:LYS:HE3	2.21	0.55
1:D:91:ILE:HD12	1:D:91:ILE:N	2.21	0.55
1:D:206:GLU:HB2	3:D:5155:HOH:O	2.06	0.55
1:A:160:ILE:HD12	1:A:245:ILE:HG12	1.89	0.54
1:D:190:LYS:HE3	3:D:5154:HOH:O	2.07	0.54
1:C:313:TYR:O	1:C:317:THR:HG23	2.07	0.54
1:D:144:CYS:SG	1:D:146:VAL:HG22	2.48	0.54
1:D:13:GLY:O	1:D:14:GLU:HB3	2.08	0.54
1:D:218:GLY:HA2	1:D:223:LYS:HB2	1.90	0.53
1:D:190:LYS:HZ1	2:D:4004:NAP:H4B	1.72	0.53
1:A:194:ILE:HG12	1:B:318:GLU:HG2	1.90	0.53
1:D:193:PRO:O	1:D:197:GLU:HG2	2.08	0.53
1:A:194:ILE:CG1	1:B:318:GLU:HG2	2.39	0.53
1:A:179:LYS:HG2	1:A:180:VAL:N	2.24	0.53
1:A:108:ARG:HH12	1:A:109:LYS:HE3	1.73	0.52
1:A:108:ARG:CZ	3:A:5156:HOH:O	2.56	0.52
1:B:163:GLY:C	1:B:191:ALA:HB2	2.30	0.52
1:C:171:GLU:HG3	1:D:313:TYR:OH	2.10	0.52
1:C:162:GLY:O	1:C:190:LYS:HD3	2.09	0.52
1:C:214:LYS:NZ	1:C:235:ILE:HD12	2.25	0.52
1:A:161:GLY:CA	3:A:5067:HOH:O	2.57	0.52
1:D:160:ILE:HD13	1:D:213:VAL:HG21	1.91	0.51
1:D:125:ARG:HH12	1:D:127:LYS:HG2	1.75	0.51
1:C:190:LYS:CD	1:C:190:LYS:H	2.18	0.51
1:B:160:ILE:HD13	1:B:213:VAL:HG21	1.92	0.51
1:B:270:LYS:HE3	3:B:5269:HOH:O	2.09	0.51
1:C:137:ALA:O	1:C:139:ARG:HG3	2.11	0.51
1:D:249:PHE:CD1	1:D:296:ARG:NH1	2.79	0.51
1:D:214:LYS:HD2	1:D:228:GLU:HB3	1.91	0.50
1:C:162:GLY:H	1:C:190:LYS:HZ1	1.58	0.50
1:A:183:ILE:HD13	1:A:227:VAL:HG21	1.94	0.50
1:B:232:THR:C	1:B:234:GLU:H	2.15	0.50
1:C:180:VAL:HB	1:C:205:VAL:HG22	1.94	0.50
1:A:156:VAL:H	1:A:241:ASN:ND2	2.09	0.49
1:C:293:LEU:HD13	1:C:294:GLY:N	2.28	0.49
1:B:107:LYS:NZ	3:B:5015:HOH:O	2.22	0.49
1:C:162:GLY:C	1:C:190:LYS:HE2	2.33	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:125:ARG:HH12	1:B:127:LYS:HD3	1.76	0.49
1:C:184:HIS:CE1	1:C:190:LYS:HZ3	2.30	0.49
1:B:295:PHE:N	3:B:5127:HOH:O	2.45	0.49
1:D:125:ARG:NH1	1:D:127:LYS:HG2	2.28	0.48
1:B:16:PHE:O	1:B:114:ALA:HA	2.13	0.48
1:A:247:ILE:HG21	3:A:5057:HOH:O	2.13	0.48
1:A:23:LEU:HG	1:A:48:PRO:HA	1.95	0.48
1:C:163:GLY:C	1:C:191:ALA:HB2	2.34	0.48
1:C:97:ASN:C	1:C:97:ASN:HD22	2.16	0.48
1:C:214:LYS:HZ2	1:C:235:ILE:HG21	1.78	0.48
1:D:160:ILE:HD11	1:D:213:VAL:HG21	1.96	0.48
1:C:19:ILE:HG13	1:C:114:ALA:HB2	1.95	0.48
1:A:88:LEU:HD11	1:A:109:LYS:HD2	1.91	0.48
1:A:211:SER:HB3	1:A:227:VAL:CG1	2.43	0.48
1:D:313:TYR:O	1:D:317:THR:HG23	2.14	0.48
1:A:131:PRO:HD2	1:A:214:LYS:O	2.15	0.47
1:C:10:VAL:C	1:C:11:LYS:HD2	2.34	0.47
1:B:125:ARG:NH2	1:B:127:LYS:HD3	2.29	0.47
1:B:199:VAL:HG12	1:B:205:VAL:HG11	1.96	0.47
1:B:45:GLY:O	1:B:89:LEU:HA	2.14	0.47
1:C:126:ARG:HD2	1:C:247:ILE:O	2.14	0.47
1:C:123:VAL:HG23	1:C:249:PHE:CD2	2.49	0.47
1:D:190:LYS:HZ3	2:D:4004:NAP:H4B	1.81	0.46
1:D:190:LYS:HB3	1:D:190:LYS:HE3	1.79	0.46
1:D:123:VAL:HG12	1:D:251:PRO:HA	1.98	0.46
1:D:45:GLY:O	1:D:89:LEU:HA	2.15	0.46
1:A:46:GLU:HB3	2:A:4005:NAP:O3X	2.15	0.46
1:D:126:ARG:HD2	1:D:247:ILE:O	2.16	0.46
1:B:263:THR:HA	1:B:268:TYR:O	2.16	0.46
1:C:184:HIS:NE2	1:C:186:ARG:HB2	2.30	0.46
1:C:45:GLY:O	1:C:89:LEU:HA	2.16	0.46
1:D:185:ARG:O	1:D:210:ASN:HA	2.16	0.46
1:C:190:LYS:NZ	2:C:4003:NAP:O2B	2.43	0.46
1:D:313:TYR:CE1	1:D:317:THR:HG21	2.51	0.46
1:B:225:VAL:HG22	1:B:240:VAL:CG2	2.46	0.46
1:A:160:ILE:CG2	3:A:5057:HOH:O	2.63	0.45
1:A:19:ILE:HG13	1:A:114:ALA:HB2	1.98	0.45
1:D:190:LYS:HE2	2:D:4004:NAP:O3B	2.16	0.45
1:C:125:ARG:NH1	1:C:126:ARG:O	2.49	0.45
1:B:98:ARG:HD2	3:B:5210:HOH:O	2.16	0.45
1:C:46:GLU:HB3	2:C:4007:NAP:O3X	2.16	0.45
1:A:196:VAL:O	1:A:200:LYS:HB2	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:163:GLY:CA	1:C:190:LYS:HE2	2.46	0.45
1:B:94:LYS:HD2	1:B:259:ASN:OD1	2.17	0.45
1:B:69:ALA:O	1:B:73:ILE:HG13	2.16	0.45
1:B:211:SER:HB3	1:B:227:VAL:CG1	2.46	0.45
1:C:217:LYS:HB2	1:C:224:GLN:HG3	1.99	0.45
1:C:130:VAL:HB	1:C:214:LYS:O	2.17	0.45
1:D:98:ARG:HG2	1:D:98:ARG:O	2.16	0.45
1:C:171:GLU:OE1	1:C:198:THR:HG22	2.16	0.45
1:D:13:GLY:O	1:D:14:GLU:CB	2.64	0.45
2:A:4001:NAP:H3D	2:A:4001:NAP:O2N	2.17	0.44
1:D:191:ALA:O	1:D:192:GLN:C	2.56	0.44
1:B:77:ASN:O	1:B:81:GLU:HG2	2.16	0.44
1:A:77:ASN:O	1:A:81:GLU:HG2	2.16	0.44
1:C:95:ILE:HD13	1:C:117:VAL:HG11	1.99	0.44
1:B:108:ARG:O	1:B:110:GLY:N	2.50	0.44
1:B:190:LYS:HE3	2:B:4002:NAP:C4B	2.41	0.44
1:D:139:ARG:NH1	3:D:5274:HOH:O	2.49	0.44
1:B:194:ILE:HG23	1:B:195:TYR:N	2.33	0.44
1:C:136:PHE:HZ	1:C:218:GLY:O	2.00	0.44
1:C:292:TRP:CE2	1:D:307:VAL:HG21	2.53	0.44
1:B:98:ARG:C	1:B:100:ASP:N	2.71	0.44
1:D:97:ASN:C	1:D:99:GLY:H	2.20	0.44
1:A:160:ILE:HG21	3:A:5057:HOH:O	2.18	0.43
1:D:19:ILE:HG13	1:D:114:ALA:HB2	2.01	0.43
1:D:13:GLY:HA3	1:D:111:GLU:O	2.18	0.43
1:C:162:GLY:HA3	1:C:190:LYS:HZ3	1.84	0.43
1:B:226:VAL:HG22	1:B:237:GLU:CG	2.47	0.43
1:D:229:ASN:C	1:D:231:LYS:H	2.22	0.43
1:D:16:PHE:CE2	1:D:42:LEU:HB2	2.54	0.43
1:A:219:ASP:OD2	1:A:220:LYS:HE2	2.18	0.43
1:A:41:THR:O	1:A:86:PRO:HD2	2.17	0.43
1:C:227:VAL:CG1	1:C:228:GLU:N	2.82	0.43
1:D:91:ILE:HD13	1:D:108:ARG:NH1	2.34	0.43
1:C:16:PHE:O	1:C:114:ALA:HA	2.19	0.43
1:D:230:LEU:C	1:D:231:LYS:HG3	2.39	0.42
1:A:299:ILE:HG23	1:A:300:THR:N	2.34	0.42
1:C:162:GLY:CA	1:C:190:LYS:HZ3	2.33	0.42
1:B:46:GLU:HB3	2:B:4006:NAP:O3X	2.19	0.42
1:C:194:ILE:HG13	1:D:318:GLU:HG2	2.01	0.42
1:D:16:PHE:O	1:D:114:ALA:HA	2.19	0.42
1:A:294:GLY:HA3	2:A:4001:NAP:C1D	2.49	0.42
1:D:225:VAL:HG13	1:D:240:VAL:CG2	2.46	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:16:PHE:O	1:A:114:ALA:HA	2.20	0.42
1:C:190:LYS:HE3	2:C:4003:NAP:H4B	1.98	0.42
1:C:93:GLU:CD	1:C:107:LYS:HA	2.40	0.42
1:D:219:ASP:OD1	1:D:223:LYS:HE3	2.20	0.42
1:C:150:PRO:HG3	1:C:176:TYR:CZ	2.54	0.42
2:C:4003:NAP:H52A	3:C:5113:HOH:O	2.19	0.42
1:D:137:ALA:C	1:D:139:ARG:H	2.22	0.42
1:B:219:ASP:HB3	1:B:220:LYS:H	1.67	0.41
1:A:182:LEU:HD23	1:A:207:PHE:CE1	2.55	0.41
1:A:263:THR:HA	1:A:268:TYR:O	2.20	0.41
1:C:212:VAL:HG22	1:C:230:LEU:HD21	2.02	0.41
1:D:125:ARG:HD2	1:D:143:TYR:CD1	2.55	0.41
1:B:160:ILE:HD11	1:B:213:VAL:HG21	2.02	0.41
1:C:227:VAL:HG12	1:C:228:GLU:H	1.85	0.41
1:B:146:VAL:HG12	1:B:172:ILE:CD1	2.50	0.41
1:C:162:GLY:C	1:C:190:LYS:CE	2.89	0.41
1:D:295:PHE:N	3:D:5058:HOH:O	2.53	0.41
1:B:253:THR:O	1:B:257:LYS:HG3	2.20	0.41
1:D:98:ARG:O	1:D:100:ASP:N	2.53	0.41
1:D:168:GLU:HB2	1:D:195:TYR:CE2	2.48	0.41
1:A:313:TYR:CE1	1:A:317:THR:HG21	2.56	0.41
1:B:11:LYS:O	1:B:12:PRO:C	2.56	0.41
1:C:247:ILE:HB	2:C:4003:NAP:C8A	2.51	0.41
1:A:318:GLU:HG2	1:B:194:ILE:CG1	2.50	0.41
1:B:65:ILE:O	1:B:66:GLU:C	2.59	0.41
1:C:38:MET:HG2	1:D:176:TYR:CE2	2.56	0.41
1:D:179:LYS:HE3	3:D:5155:HOH:O	2.21	0.41
1:C:299:ILE:HG23	1:C:300:THR:N	2.35	0.41
1:D:276:ARG:HG2	1:D:283:PHE:CE2	2.56	0.41
1:C:236:LYS:HE2	1:C:238:LEU:HD21	2.02	0.41
1:B:231:LYS:HE2	1:B:231:LYS:HB3	1.79	0.41
1:A:228:GLU:HB2	1:A:235:ILE:CD1	2.51	0.40
1:B:179:LYS:HE3	1:B:181:TYR:CE1	2.55	0.40
1:D:46:GLU:HB3	2:D:4008:NAP:O3X	2.21	0.40
1:C:193:PRO:O	1:C:197:GLU:HG2	2.21	0.40
1:A:176:TYR:CZ	1:B:38:MET:HG3	2.56	0.40
1:A:179:LYS:HG2	1:A:180:VAL:H	1.86	0.40
1:C:253:THR:CG2	1:C:257:LYS:HE3	2.49	0.40
1:D:77:ASN:CB	3:D:5137:HOH:O	2.70	0.40
1:B:296:ARG:HG3	1:B:296:ARG:HH11	1.87	0.40
1:A:160:ILE:CD1	1:A:213:VAL:HG21	2.52	0.40
1:A:125:ARG:HH11	1:A:125:ARG:HG2	1.87	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:163:GLY:C	1:D:191:ALA:HB2	2.42	0.40
1:D:137:ALA:C	1:D:139:ARG:N	2.74	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	304/323 (94%)	295 (97%)	9 (3%)	0	100	100
1	B	305/323 (94%)	288 (94%)	14 (5%)	3 (1%)	22	9
1	C	303/323 (94%)	293 (97%)	10 (3%)	0	100	100
1	D	294/323 (91%)	278 (95%)	14 (5%)	2 (1%)	30	15
All	All	1206/1292 (93%)	1154 (96%)	47 (4%)	5 (0%)	43	30

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	109	LYS
1	B	14	GLU
1	B	233	GLY
1	D	14	GLU
1	D	230	LEU

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	253/267 (95%)	250 (99%)	3 (1%)	82	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	254/267 (95%)	248 (98%)	6 (2%)	61	51
1	C	252/267 (94%)	248 (98%)	4 (2%)	75	69
1	D	243/267 (91%)	240 (99%)	3 (1%)	82	79
All	All	1002/1068 (94%)	986 (98%)	16 (2%)	75	69

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	LYS
1	A	134	GLN
1	A	293	LEU
1	B	109	LYS
1	B	125	ARG
1	B	128	LEU
1	B	190	LYS
1	B	225	VAL
1	B	293	LEU
1	C	97	ASN
1	C	155	ARG
1	C	190	LYS
1	C	265	THR
1	D	108	ARG
1	D	187	ASP
1	D	296	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	GLN
1	A	241	ASN
1	A	266	ASN
1	B	241	ASN
1	B	266	ASN
1	B	297	GLN
1	C	97	ASN
1	C	184	HIS
1	C	192	GLN
1	C	241	ASN
1	D	241	ASN
1	D	297	GLN

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	4001	-	52,52,52	1.47	6 (11%)	80,80,80	1.37	11 (13%)
2	NAP	A	4005	-	33,33,52	2.22	6 (18%)	52,52,80	1.26	9 (17%)
2	NAP	B	4002	-	52,52,52	1.43	8 (15%)	80,80,80	1.45	11 (13%)
2	NAP	B	4006	-	33,33,52	2.00	6 (18%)	52,52,80	1.25	6 (11%)
2	NAP	C	4003	-	52,52,52	1.46	6 (11%)	80,80,80	1.38	10 (12%)
2	NAP	C	4007	-	33,33,52	2.14	6 (18%)	52,52,80	1.39	5 (9%)
2	NAP	D	4004	-	52,52,52	1.50	6 (11%)	80,80,80	1.46	10 (12%)
2	NAP	D	4008	-	30,32,52	1.48	4 (13%)	45,49,80	1.45	5 (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	4001	-	-	0/35/67/67	0/3/5/5
2	NAP	A	4005	-	-	0/21/37/67	0/1/3/5
2	NAP	B	4002	-	-	0/35/67/67	0/3/5/5
2	NAP	B	4006	-	-	0/21/37/67	0/1/3/5
2	NAP	C	4003	-	-	0/35/67/67	0/3/5/5
2	NAP	C	4007	-	-	0/21/37/67	0/1/3/5
2	NAP	D	4004	-	-	0/35/67/67	0/3/5/5
2	NAP	D	4008	-	-	0/18/36/67	0/1/3/5

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4005	NAP	PN-O5D	8.88	1.66	1.51
2	C	4007	NAP	PN-O5D	7.75	1.65	1.51
2	B	4006	NAP	PN-O5D	7.60	1.64	1.51
2	D	4004	NAP	C3N-C7N	5.47	1.59	1.50
2	A	4001	NAP	C3N-C7N	5.44	1.59	1.50
2	C	4003	NAP	C3N-C7N	5.20	1.59	1.50
2	A	4001	NAP	C2N-N1N	5.20	1.42	1.35
2	D	4004	NAP	C2N-N1N	5.18	1.41	1.35
2	C	4003	NAP	C2N-N1N	5.05	1.41	1.35
2	B	4002	NAP	C3N-C7N	4.95	1.59	1.50
2	C	4007	NAP	P2B-O2X	-4.70	1.37	1.54
2	A	4005	NAP	P2B-O2B	4.53	1.73	1.59
2	A	4005	NAP	P2B-O2X	-4.47	1.38	1.54
2	B	4006	NAP	P2B-O2X	-4.46	1.38	1.54
2	D	4008	NAP	P2B-O2X	-4.22	1.39	1.54
2	B	4002	NAP	C2N-N1N	4.05	1.40	1.35
2	C	4007	NAP	PN-O1N	-4.05	1.44	1.51
2	C	4007	NAP	P2B-O2B	3.77	1.71	1.59
2	B	4006	NAP	P2B-O2B	3.39	1.70	1.59
2	D	4008	NAP	P2B-O2B	3.23	1.69	1.59
2	B	4006	NAP	PA-O3	3.07	1.65	1.59
2	A	4005	NAP	PN-O1N	-2.93	1.46	1.51
2	B	4002	NAP	C8A-N7A	-2.93	1.28	1.34
2	D	4004	NAP	O4B-C1B	2.84	1.45	1.41
2	C	4003	NAP	C8A-N7A	-2.79	1.29	1.34
2	D	4004	NAP	C8A-N7A	-2.76	1.29	1.34
2	C	4007	NAP	C4A-N3A	2.75	1.39	1.35
2	A	4001	NAP	C8A-N7A	-2.74	1.29	1.34
2	B	4002	NAP	C6N-N1N	2.57	1.42	1.35
2	D	4008	NAP	PN-O1N	2.56	1.49	1.46
2	D	4008	NAP	C8A-N9A	2.47	1.40	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4001	NAP	C6N-N1N	2.44	1.42	1.35
2	C	4003	NAP	O4D-C1D	2.42	1.45	1.41
2	B	4006	NAP	C8A-N7A	-2.40	1.29	1.34
2	C	4003	NAP	C6N-N1N	2.39	1.42	1.35
2	D	4004	NAP	C6N-N1N	2.36	1.42	1.35
2	B	4002	NAP	PA-O3	2.34	1.64	1.59
2	B	4002	NAP	P2B-O3X	-2.33	1.46	1.54
2	A	4001	NAP	O4D-C1D	2.24	1.44	1.41
2	A	4005	NAP	PN-O2N	-2.21	1.48	1.51
2	A	4005	NAP	C4A-N3A	2.20	1.39	1.35
2	C	4003	NAP	O4B-C1B	2.19	1.44	1.41
2	B	4006	NAP	O4B-C1B	2.18	1.44	1.41
2	C	4007	NAP	PA-O2A	-2.18	1.45	1.55
2	D	4004	NAP	O4D-C1D	2.13	1.44	1.41
2	A	4001	NAP	P2B-O2X	-2.12	1.46	1.54
2	B	4002	NAP	C4A-N3A	2.12	1.38	1.35
2	B	4002	NAP	O4D-C1D	2.12	1.44	1.41

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	4008	NAP	O4B-C1B-C2B	-5.62	101.69	106.95
2	B	4002	NAP	O4D-C1D-N1N	5.41	113.49	107.95
2	C	4007	NAP	O4B-C1B-C2B	-4.92	102.35	106.95
2	C	4003	NAP	C3N-C7N-N7N	4.71	123.13	117.77
2	A	4001	NAP	C3N-C7N-N7N	4.60	123.01	117.77
2	D	4004	NAP	C3N-C7N-N7N	4.45	122.84	117.77
2	D	4004	NAP	O4B-C1B-N9A	4.42	112.55	108.44
2	B	4002	NAP	C3N-C7N-N7N	4.10	122.44	117.77
2	D	4004	NAP	O4D-C1D-N1N	4.04	112.08	107.95
2	B	4002	NAP	O4B-C1B-N9A	3.93	112.09	108.44
2	D	4004	NAP	C8A-N9A-C4A	-3.57	104.17	106.90
2	C	4003	NAP	O4B-C1B-N9A	3.39	111.59	108.44
2	A	4001	NAP	O4B-C1B-N9A	3.31	111.52	108.44
2	D	4008	NAP	O2X-P2B-O1X	3.28	121.17	110.44
2	B	4006	NAP	O2X-P2B-O1X	3.26	121.09	110.44
2	A	4001	NAP	C8A-N9A-C4A	-3.26	104.41	106.90
2	A	4005	NAP	O2X-P2B-O1X	3.25	121.08	110.44
2	C	4003	NAP	C8A-N9A-C4A	-3.21	104.45	106.90
2	C	4007	NAP	O2X-P2B-O1X	3.18	120.83	110.44
2	C	4003	NAP	O7N-C7N-C3N	-3.16	116.01	119.58
2	D	4004	NAP	C4B-O4B-C1B	-3.10	106.38	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4001	NAP	C6N-N1N-C2N	-3.07	118.57	122.04
2	B	4002	NAP	C4B-O4B-C1B	-3.05	106.43	109.75
2	C	4003	NAP	O4D-C1D-N1N	3.04	111.06	107.95
2	A	4001	NAP	C4B-O4B-C1B	-3.04	106.45	109.75
2	B	4006	NAP	C4B-O4B-C1B	-2.99	106.50	109.75
2	D	4004	NAP	O7N-C7N-C3N	-2.93	116.27	119.58
2	A	4001	NAP	O7N-C7N-C3N	-2.90	116.31	119.58
2	C	4007	NAP	O3X-P2B-O2B	-2.90	98.75	107.09
2	D	4008	NAP	O3X-P2B-O2B	-2.84	98.91	107.09
2	C	4003	NAP	C6N-N1N-C2N	-2.84	118.84	122.04
2	B	4006	NAP	O3X-P2B-O2B	-2.81	99.00	107.09
2	C	4003	NAP	C4B-O4B-C1B	-2.78	106.73	109.75
2	B	4006	NAP	O4B-C1B-C2B	-2.78	104.35	106.95
2	D	4008	NAP	C8A-N9A-C4A	-2.76	104.79	106.90
2	B	4002	NAP	C6N-N1N-C2N	-2.75	118.93	122.04
2	D	4004	NAP	C6N-N1N-C2N	-2.75	118.94	122.04
2	A	4001	NAP	O4D-C1D-N1N	2.70	110.71	107.95
2	D	4004	NAP	C4A-C5A-N7A	2.66	111.80	109.52
2	A	4005	NAP	O3X-P2B-O2B	-2.66	99.43	107.09
2	B	4002	NAP	O7N-C7N-C3N	-2.65	116.59	119.58
2	C	4003	NAP	C3D-C2D-C1D	2.62	105.01	100.91
2	A	4005	NAP	O2N-PN-O1N	2.53	118.56	112.73
2	A	4001	NAP	C3D-C2D-C1D	2.53	104.87	100.91
2	C	4003	NAP	C4A-C5A-N7A	2.52	111.68	109.52
2	B	4002	NAP	C3D-C2D-C1D	2.50	104.82	100.91
2	A	4005	NAP	O4B-C1B-C2B	-2.50	104.61	106.95
2	B	4002	NAP	C4A-C5A-N7A	2.46	111.63	109.52
2	C	4003	NAP	O5D-C5D-C4D	2.45	117.92	108.94
2	B	4002	NAP	C8A-N9A-C4A	-2.45	105.03	106.90
2	D	4004	NAP	C3D-C2D-C1D	2.45	104.74	100.91
2	A	4005	NAP	C4A-C5A-N7A	2.41	111.59	109.52
2	A	4001	NAP	O5D-C5D-C4D	2.34	117.51	108.94
2	A	4001	NAP	C4A-C5A-N7A	2.33	111.52	109.52
2	B	4006	NAP	C4A-C5A-N7A	2.33	111.52	109.52
2	D	4004	NAP	O5D-C5D-C4D	2.30	117.38	108.94
2	A	4005	NAP	O5D-PN-O1N	-2.27	107.50	112.73
2	B	4002	NAP	O4B-C1B-C2B	2.27	109.07	106.95
2	A	4005	NAP	C8A-N9A-C4A	-2.27	105.17	106.90
2	B	4002	NAP	O3B-C3B-C4B	2.21	117.58	111.08
2	C	4007	NAP	O2N-PN-O1N	2.19	117.77	112.73
2	C	4007	NAP	C4A-C5A-N7A	2.18	111.39	109.52
2	B	4006	NAP	C8A-N9A-C4A	-2.15	105.26	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	4008	NAP	C4A-C5A-N7A	2.08	111.31	109.52
2	A	4001	NAP	C1B-N9A-C4A	2.02	130.12	126.64
2	A	4005	NAP	C4B-O4B-C1B	-2.01	107.56	109.75
2	A	4005	NAP	O2B-C2B-C3B	2.01	119.38	111.54

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	308/323 (95%)	0.21	8 (2%) 53 61	8, 22, 45, 59	0
1	B	309/323 (95%)	0.44	15 (4%) 28 35	9, 25, 48, 70	0
1	C	307/323 (95%)	0.32	19 (6%) 20 25	8, 21, 55, 68	0
1	D	298/323 (92%)	0.42	28 (9%) 9 11	7, 22, 57, 71	0
All	All	1222/1292 (94%)	0.35	70 (5%) 22 29	7, 23, 52, 71	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	194	ILE	6.8
1	D	219	ASP	6.6
1	A	98	ARG	4.5
1	B	98	ARG	4.2
1	D	195	TYR	4.2
1	B	194	ILE	3.9
1	B	13	GLY	3.8
1	D	13	GLY	3.6
1	B	108	ARG	3.4
1	C	230	LEU	3.3
1	A	220	LYS	3.3
1	B	11	LYS	3.3
1	D	200	LYS	3.2
1	C	232	THR	3.2
1	D	100	ASP	3.2
1	D	188	THR	3.1
1	D	98	ARG	3.1
1	A	219	ASP	3.1
1	D	220	LYS	3.1
1	D	138	GLY	3.0
1	C	186	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	99	GLY	2.9
1	C	214	LYS	2.9
1	B	12	PRO	2.9
1	C	220	LYS	2.9
1	D	54	GLU	2.9
1	D	190	LYS	2.8
1	C	193	PRO	2.8
1	C	221	VAL	2.7
1	A	108	ARG	2.7
1	D	201	LYS	2.7
1	C	234	GLU	2.7
1	A	186	ARG	2.7
1	D	186	ARG	2.6
1	D	192	GLN	2.6
1	C	249	PHE	2.6
1	C	235	ILE	2.6
1	C	190	LYS	2.5
1	D	129	GLY	2.5
1	C	233	GLY	2.5
1	C	127	LYS	2.5
1	D	127	LYS	2.4
1	C	231	LYS	2.4
1	B	183	ILE	2.4
1	C	187	ASP	2.4
1	B	186	ARG	2.4
1	D	155	ARG	2.4
1	D	139	ARG	2.4
1	B	125	ARG	2.3
1	D	160	ILE	2.3
1	B	231	LYS	2.3
1	B	100	ASP	2.3
1	C	197	GLU	2.3
1	C	125	ARG	2.3
1	A	231	LYS	2.3
1	A	187	ASP	2.2
1	D	137	ALA	2.2
1	C	54	GLU	2.2
1	B	160	ILE	2.2
1	B	235	ILE	2.2
1	D	193	PRO	2.2
1	D	159	VAL	2.2
1	C	219	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	21	VAL	2.1
1	D	134	GLN	2.1
1	D	207	PHE	2.1
1	A	197	GLU	2.1
1	B	107	LYS	2.1
1	D	197	GLU	2.1
1	D	230	LEU	2.1

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	NAP	A	4001	48/48	0.20	1.08	36,48,77,79	0
2	NAP	D	4008	30/48	0.14	0.73	11,18,53,55	0
2	NAP	A	4005	31/48	0.13	0.65	8,16,43,46	0
2	NAP	D	4004	48/48	0.20	0.35	33,54,76,79	0
2	NAP	C	4007	31/48	0.12	0.32	10,14,33,37	0
2	NAP	B	4002	48/48	0.16	0.17	28,39,70,72	0
2	NAP	C	4003	48/48	0.17	-0.04	33,42,74,76	0
2	NAP	B	4006	31/48	0.12	-0.20	13,25,48,50	0

6.5 Other polymers ⓘ

There are no such residues in this entry.