



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:34 PM GMT

PDB ID : 4CMJ
Title : Crystal structure of pteridine reductase 1 (PTR1) from Trypanosoma brucei
in ternary complex with cofactor and inhibitor
Authors : Barrack, K.L.; Hunter, W.N.
Deposited on : 2014-01-16
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

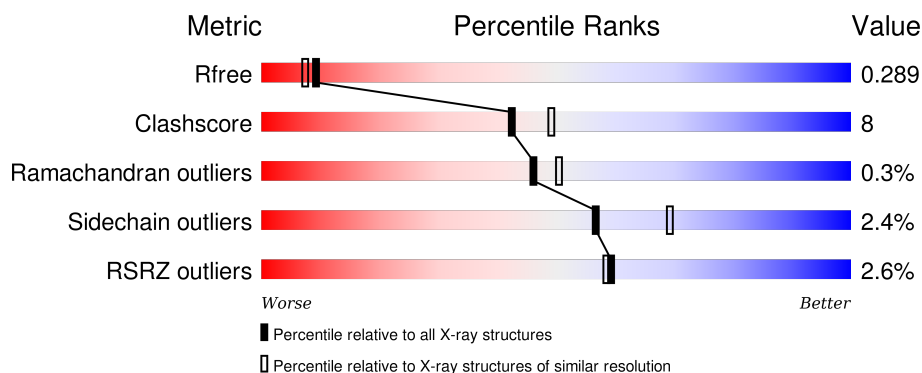
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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. 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	288	 2% 73% 14% 13%
1	B	288	 2% 72% 14% • 13%
1	C	288	 2% 70% 17% 13%
1	D	288	 3% 70% 15% • 14%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8112 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 PTERIDINE REDUCTASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	S	0	0	0
			1869	1173	330	355	11			
1	B	251	Total	C	N	O	S	0	1	0
			1877	1179	332	355	11			
1	C	251	Total	C	N	O	S	0	0	0
			1869	1173	330	355	11			
1	D	249	Total	C	N	O	S	0	0	0
			1854	1165	327	351	11			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP O76290
A	-18	GLY	-	EXPRESSION TAG	UNP O76290
A	-17	SER	-	EXPRESSION TAG	UNP O76290
A	-16	SER	-	EXPRESSION TAG	UNP O76290
A	-15	HIS	-	EXPRESSION TAG	UNP O76290
A	-14	HIS	-	EXPRESSION TAG	UNP O76290
A	-13	HIS	-	EXPRESSION TAG	UNP O76290
A	-12	HIS	-	EXPRESSION TAG	UNP O76290
A	-11	HIS	-	EXPRESSION TAG	UNP O76290
A	-10	HIS	-	EXPRESSION TAG	UNP O76290
A	-9	SER	-	EXPRESSION TAG	UNP O76290
A	-8	SER	-	EXPRESSION TAG	UNP O76290
A	-7	GLY	-	EXPRESSION TAG	UNP O76290
A	-6	LEU	-	EXPRESSION TAG	UNP O76290
A	-5	VAL	-	EXPRESSION TAG	UNP O76290
A	-4	PRO	-	EXPRESSION TAG	UNP O76290
A	-3	ARG	-	EXPRESSION TAG	UNP O76290
A	-2	GLY	-	EXPRESSION TAG	UNP O76290
A	-1	SER	-	EXPRESSION TAG	UNP O76290
A	0	HIS	-	EXPRESSION TAG	UNP O76290
B	-19	MET	-	EXPRESSION TAG	UNP O76290

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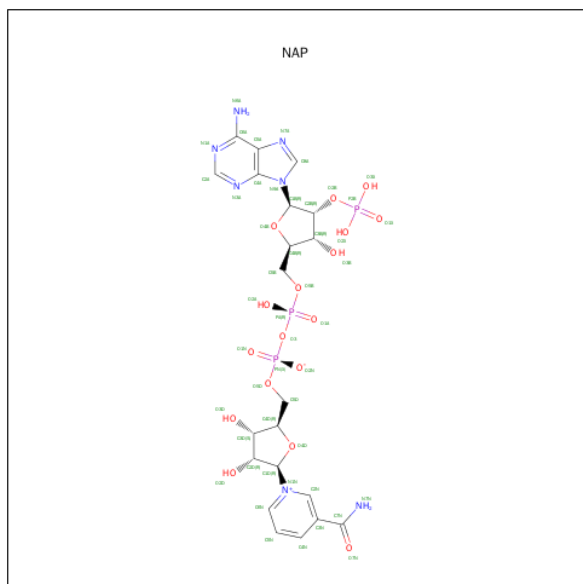
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	EXPRESSION TAG	UNP O76290
B	-17	SER	-	EXPRESSION TAG	UNP O76290
B	-16	SER	-	EXPRESSION TAG	UNP O76290
B	-15	HIS	-	EXPRESSION TAG	UNP O76290
B	-14	HIS	-	EXPRESSION TAG	UNP O76290
B	-13	HIS	-	EXPRESSION TAG	UNP O76290
B	-12	HIS	-	EXPRESSION TAG	UNP O76290
B	-11	HIS	-	EXPRESSION TAG	UNP O76290
B	-10	HIS	-	EXPRESSION TAG	UNP O76290
B	-9	SER	-	EXPRESSION TAG	UNP O76290
B	-8	SER	-	EXPRESSION TAG	UNP O76290
B	-7	GLY	-	EXPRESSION TAG	UNP O76290
B	-6	LEU	-	EXPRESSION TAG	UNP O76290
B	-5	VAL	-	EXPRESSION TAG	UNP O76290
B	-4	PRO	-	EXPRESSION TAG	UNP O76290
B	-3	ARG	-	EXPRESSION TAG	UNP O76290
B	-2	GLY	-	EXPRESSION TAG	UNP O76290
B	-1	SER	-	EXPRESSION TAG	UNP O76290
B	0	HIS	-	EXPRESSION TAG	UNP O76290
C	-19	MET	-	EXPRESSION TAG	UNP O76290
C	-18	GLY	-	EXPRESSION TAG	UNP O76290
C	-17	SER	-	EXPRESSION TAG	UNP O76290
C	-16	SER	-	EXPRESSION TAG	UNP O76290
C	-15	HIS	-	EXPRESSION TAG	UNP O76290
C	-14	HIS	-	EXPRESSION TAG	UNP O76290
C	-13	HIS	-	EXPRESSION TAG	UNP O76290
C	-12	HIS	-	EXPRESSION TAG	UNP O76290
C	-11	HIS	-	EXPRESSION TAG	UNP O76290
C	-10	HIS	-	EXPRESSION TAG	UNP O76290
C	-9	SER	-	EXPRESSION TAG	UNP O76290
C	-8	SER	-	EXPRESSION TAG	UNP O76290
C	-7	GLY	-	EXPRESSION TAG	UNP O76290
C	-6	LEU	-	EXPRESSION TAG	UNP O76290
C	-5	VAL	-	EXPRESSION TAG	UNP O76290
C	-4	PRO	-	EXPRESSION TAG	UNP O76290
C	-3	ARG	-	EXPRESSION TAG	UNP O76290
C	-2	GLY	-	EXPRESSION TAG	UNP O76290
C	-1	SER	-	EXPRESSION TAG	UNP O76290
C	0	HIS	-	EXPRESSION TAG	UNP O76290
D	-19	MET	-	EXPRESSION TAG	UNP O76290
D	-18	GLY	-	EXPRESSION TAG	UNP O76290
D	-17	SER	-	EXPRESSION TAG	UNP O76290

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	EXPRESSION TAG	UNP O76290
D	-15	HIS	-	EXPRESSION TAG	UNP O76290
D	-14	HIS	-	EXPRESSION TAG	UNP O76290
D	-13	HIS	-	EXPRESSION TAG	UNP O76290
D	-12	HIS	-	EXPRESSION TAG	UNP O76290
D	-11	HIS	-	EXPRESSION TAG	UNP O76290
D	-10	HIS	-	EXPRESSION TAG	UNP O76290
D	-9	SER	-	EXPRESSION TAG	UNP O76290
D	-8	SER	-	EXPRESSION TAG	UNP O76290
D	-7	GLY	-	EXPRESSION TAG	UNP O76290
D	-6	LEU	-	EXPRESSION TAG	UNP O76290
D	-5	VAL	-	EXPRESSION TAG	UNP O76290
D	-4	PRO	-	EXPRESSION TAG	UNP O76290
D	-3	ARG	-	EXPRESSION TAG	UNP O76290
D	-2	GLY	-	EXPRESSION TAG	UNP O76290
D	-1	SER	-	EXPRESSION TAG	UNP O76290
D	0	HIS	-	EXPRESSION TAG	UNP O76290

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



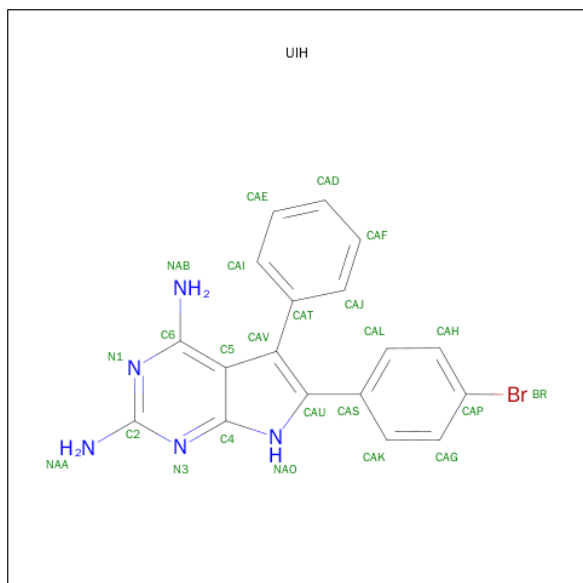
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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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 6-(4-BROMOPHENYL)-5-PHENYL-7H-PYRROLO[2,3-D]PYRIMIDINE-2,4-DIAMINE (three-letter code: UIH) (formula: C₁₈H₁₄BrN₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	Br	C	N	0	0
			24	1	18	5		
3	B	1	Total	Br	C	N	0	0
			24	1	18	5		
3	C	1	Total	Br	C	N	0	0
			24	1	18	5		
3	D	1	Total	Br	C	N	0	0
			24	1	18	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	108	Total	O	0	0
			108	108		
4	B	104	Total	O	0	0
			104	104		
4	C	84	Total	O	0	0
			84	84		

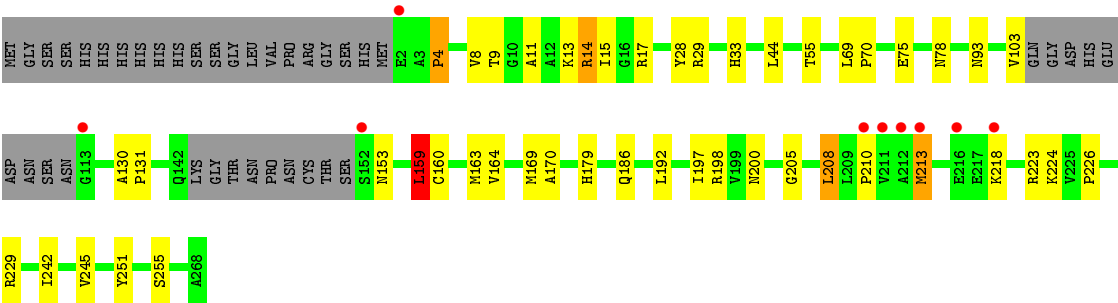
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	59	Total	O	0	0
			59	59		

- Molecule 1: PTERIDINE REDUCTASE 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.30 Å 90.20 Å 82.19 Å 90.00° 115.65° 90.00°	Depositor
Resolution (Å)	13.94 – 2.20 13.94 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.8 (13.94-2.20) 94.3 (13.94-2.20)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.20 Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.205 , 0.285 0.212 , 0.289	Depositor DCC
R_{free} test set	2348 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	14.6	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 33.9	EDS
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	3 of 46669 reflections (0.006%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8112	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 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: UIH, 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	0.71	0/1896	0.84	2/2572 (0.1%)
1	B	0.73	0/1907	0.87	3/2586 (0.1%)
1	C	0.67	0/1896	0.86	3/2572 (0.1%)
1	D	0.68	0/1881	0.86	3/2552 (0.1%)
All	All	0.69	0/7580	0.86	11/10282 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	ARG	NE-CZ-NH1	9.39	124.99	120.30
1	D	198	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	A	198	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	B	198	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	D	198	ARG	NE-CZ-NH1	7.43	124.01	120.30
1	C	198	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	D	159	LEU	CA-CB-CG	-6.64	100.02	115.30
1	B	159	LEU	CA-CB-CG	-6.35	100.69	115.30
1	C	198	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	B	222	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	C	229	ARG	NE-CZ-NH1	5.29	122.94	120.30

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	1869	0	1890	32	0
1	B	1877	0	1904	28	0
1	C	1869	0	1890	35	0
1	D	1854	0	1877	31	0
2	A	48	0	25	1	0
2	B	48	0	25	1	0
2	C	48	0	25	1	0
2	D	48	0	25	1	0
3	A	24	0	14	5	0
3	B	24	0	14	3	0
3	C	24	0	14	6	0
3	D	24	0	14	4	0
4	A	108	0	0	10	0
4	B	104	0	0	8	1
4	C	84	0	0	5	1
4	D	59	0	0	3	0
All	All	8112	0	7717	129	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (129) 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:197:ILE:HG23	4:A:2052:HOH:O	1.62	1.00
1:A:155:SER:HA	4:A:2052:HOH:O	1.69	0.93
3:D:1270:UIH:CAI	3:D:1270:UIH:HAL	2.01	0.90
1:B:217:GLU:HB2	4:B:2084:HOH:O	1.79	0.83
1:C:198:ARG:HD3	4:C:2044:HOH:O	1.84	0.78
1:B:66:SER:HA	4:B:2035:HOH:O	1.84	0.78
3:C:1270:UIH:HAL	3:C:1270:UIH:CAT	2.16	0.74
1:A:164:VAL:HG22	1:A:179:HIS:CD2	2.28	0.68
3:A:1270:UIH:CAT	3:A:1270:UIH:HAK	2.26	0.65
1:A:78:ASN:OD1	1:A:141:ARG:NH1	2.31	0.64
1:D:160:CYS:HB3	4:D:2040:HOH:O	1.98	0.63
1:A:93:ASN:OD1	1:A:159:LEU:HD13	2.01	0.61
1:B:206:VAL:HG22	3:B:1270:UIH:HAF	1.83	0.61
1:B:198:ARG:HD3	4:B:2057:HOH:O	1.99	0.61
1:A:140:GLN:HE22	1:C:104:GLN:H	1.48	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:TYR:CE2	1:B:232:ALA:HB2	2.37	0.59
1:A:163:MET:HG2	4:A:2056:HOH:O	2.03	0.58
1:C:232:ALA:HB2	1:D:251:TYR:CD2	2.38	0.58
1:A:172:SER:O	1:A:176:MET:HG3	2.02	0.58
1:D:169:MET:O	1:D:170:ALA:HB3	2.04	0.58
1:D:29:ARG:HG2	1:D:55:THR:HG22	1.86	0.58
3:D:1270:UIH:HAL	3:D:1270:UIH:CAT	2.33	0.57
1:D:213:MET:HB3	1:D:218:LYS:HG3	1.86	0.57
1:C:208:LEU:O	4:C:2059:HOH:O	2.18	0.56
1:C:164:VAL:HG22	1:C:179:HIS:CD2	2.40	0.55
1:A:68:VAL:HG22	4:A:2026:HOH:O	2.06	0.55
1:D:205:GLY:O	2:D:1269:NAP:H4N	2.07	0.55
1:C:97:PHE:CE2	3:C:1270:UIH:HAJ	2.42	0.55
1:D:130:ALA:HB3	1:D:131:PRO:HD3	1.88	0.54
3:D:1270:UIH:CAI	3:D:1270:UIH:CAL	2.82	0.54
1:B:164:VAL:HG22	1:B:179:HIS:CD2	2.42	0.54
1:D:153:ASN:ND2	1:D:245:VAL:O	2.40	0.54
1:C:232:ALA:HB2	1:D:251:TYR:CE2	2.42	0.54
3:A:1270:UIH:CAK	3:A:1270:UIH:CAJ	2.87	0.53
1:A:250:GLN:HE21	1:A:250:GLN:HA	1.73	0.53
1:B:140:GLN:HE22	1:B:143:LYS:HE2	1.74	0.53
1:B:24:HIS:O	1:B:52:ARG:NH2	2.42	0.53
1:D:8:VAL:CG1	1:D:11:ALA:HB2	2.40	0.52
1:A:168:CYS:SG	3:A:1270:UIH:CAG	2.97	0.52
1:C:61:ALA:HB3	1:C:76:ILE:HD11	1.91	0.52
1:C:117:GLU:HB2	4:C:2038:HOH:O	2.10	0.52
1:A:9:THR:HA	1:A:33:HIS:HB3	1.91	0.52
3:C:1270:UIH:HAL	3:C:1270:UIH:CAI	2.39	0.52
1:B:38:ALA:O	1:B:42:VAL:HG22	2.10	0.52
1:B:31:VAL:HG21	1:B:80:CYS:HB2	1.93	0.51
1:C:97:PHE:CZ	3:C:1270:UIH:HAJ	2.46	0.51
1:D:4:PRO:HB2	1:D:28:TYR:CD2	2.45	0.50
1:C:42:VAL:CG2	4:C:2016:HOH:O	2.60	0.50
1:D:223:ARG:O	1:D:229:ARG:NH1	2.42	0.49
1:A:65:ASN:HA	1:A:69:LEU:HD22	1.94	0.49
1:A:268:ALA:OXT	1:D:224:LYS:HE3	2.12	0.49
1:A:124:ILE:HG22	1:A:129:ILE:CD1	2.42	0.49
1:A:197:ILE:CG2	4:A:2052:HOH:O	2.39	0.49
3:A:1270:UIH:HAK	3:A:1270:UIH:CAJ	2.43	0.49
1:A:232:ALA:HB2	1:B:251:TYR:CE2	2.48	0.49
4:A:2066:HOH:O	1:C:191:GLU:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:PRO:HB2	1:D:28:TYR:CE2	2.49	0.48
1:C:175:ASN:ND2	4:C:2048:HOH:O	2.46	0.48
1:C:158:ASN:HB3	1:C:181:LEU:HD11	1.96	0.48
3:C:1270:UIH:CAL	3:C:1270:UIH:CAT	2.88	0.48
1:A:155:SER:CA	4:A:2052:HOH:O	2.40	0.47
1:D:9:THR:HA	1:D:33:HIS:HB3	1.96	0.47
1:C:69:LEU:N	1:C:70:PRO:CD	2.77	0.47
1:B:33:HIS:CG	1:B:34:TYR:N	2.82	0.47
1:C:159:LEU:HD22	2:C:1269:NAP:H4D	1.96	0.47
1:A:9:THR:O	1:A:93:ASN:HB3	2.15	0.47
2:B:1269:NAP:O1A	3:B:1270:UIH:N1	2.48	0.47
1:A:250:GLN:NE2	1:A:250:GLN:HA	2.29	0.47
1:C:15:ILE:HA	1:C:234:ALA:HB1	1.96	0.47
1:C:49:ASN:HA	1:C:52:ARG:O	2.14	0.47
3:C:1270:UIH:HAL	3:C:1270:UIH:CAJ	2.44	0.47
1:B:193:ALA:N	1:B:194:PRO:CD	2.78	0.46
1:A:88:ASP:O	1:A:154:LEU:HA	2.16	0.46
1:C:172:SER:O	1:C:176:MET:HG3	2.14	0.46
1:D:224:LYS:O	1:D:226:PRO:HD3	2.15	0.46
1:B:66:SER:HB3	4:B:2038:HOH:O	2.15	0.46
1:C:38:ALA:O	1:C:42:VAL:HG13	2.16	0.46
1:A:160:CYS:O	2:A:1269:NAP:H6N	2.16	0.46
3:B:1270:UIH:CAT	3:B:1270:UIH:HAK	2.46	0.45
1:C:17:ARG:NH1	1:C:44:LEU:HD13	2.31	0.45
1:D:15:ILE:HG13	4:D:2008:HOH:O	2.14	0.45
1:A:179:HIS:ND1	4:A:2067:HOH:O	2.04	0.45
1:C:86:ARG:HD3	1:C:88:ASP:OD2	2.16	0.45
1:D:200:ASN:HB3	1:D:255:SER:O	2.16	0.45
3:A:1270:UIH:CAT	3:A:1270:UIH:CAK	2.90	0.45
1:D:210:PRO:O	1:D:218:LYS:HD3	2.16	0.45
1:A:232:ALA:HB2	1:B:251:TYR:CD2	2.51	0.45
1:C:88:ASP:O	1:C:154:LEU:HA	2.16	0.45
1:D:242:ILE:HA	1:D:245:VAL:HG22	1.98	0.45
1:B:6:ALA:HB2	1:B:89:VAL:HB	1.99	0.45
1:C:9:THR:O	1:C:93:ASN:HB3	2.17	0.45
1:D:163:MET:HG3	3:D:1270:UIH:BR	2.72	0.45
1:D:69:LEU:HB3	1:D:70:PRO:HD3	1.98	0.45
1:C:266:VAL:HG12	1:C:267:HIS:O	2.17	0.44
1:B:26:THR:HG22	1:B:26:THR:O	2.17	0.44
1:A:117:GLU:HG2	1:C:67:ASN:HA	1.98	0.44
1:D:93:ASN:OD1	1:D:159:LEU:HD13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:ALA:HB3	1:C:131:PRO:HD3	1.99	0.44
1:C:33:HIS:CG	1:C:34:TYR:N	2.86	0.44
1:B:10:GLY:HA2	4:B:2005:HOH:O	2.17	0.44
1:B:140:GLN:NE2	1:B:143:LYS:HE2	2.32	0.43
1:A:4:PRO:HB2	1:A:28:TYR:CE2	2.52	0.43
1:A:130:ALA:HB3	1:A:131:PRO:HD3	1.99	0.43
1:B:11:ALA:HB3	1:B:32:ILE:HG23	2.00	0.43
1:D:103:VAL:HG12	1:D:103:VAL:O	2.18	0.43
1:D:75:GLU:HA	1:D:78:ASN:HB2	2.01	0.43
1:B:209:LEU:O	1:B:210:PRO:C	2.54	0.43
1:B:117:GLU:HG3	1:D:70:PRO:HG2	2.01	0.43
1:C:151:SER:OG	1:C:151:SER:O	2.30	0.42
1:B:227:LEU:HA	1:B:227:LEU:HD12	1.91	0.42
1:C:52:ARG:HD2	1:C:55:THR:HG21	2.01	0.42
1:A:229:ARG:NH1	4:A:2084:HOH:O	2.52	0.42
1:B:157:VAL:HG11	1:B:241:VAL:HG13	2.02	0.42
4:A:2067:HOH:O	1:C:179:HIS:ND1	2.21	0.42
1:A:161:ASP:OD1	1:A:161:ASP:C	2.57	0.42
1:B:155:SER:HA	1:B:198:ARG:O	2.20	0.42
1:B:66:SER:CB	4:B:2038:HOH:O	2.68	0.42
1:D:192:LEU:HB3	1:D:197:ILE:HB	2.02	0.42
1:D:164:VAL:HG22	1:D:179:HIS:CD2	2.54	0.42
1:B:35:HIS:CD2	1:B:62:ASP:HA	2.55	0.41
1:C:209:LEU:HD22	1:C:218:LYS:HA	2.00	0.41
1:A:120:VAL:HG11	1:C:129:ILE:HD13	2.02	0.41
4:B:2063:HOH:O	1:D:186:GLN:NE2	2.26	0.41
1:A:19:ILE:CD1	1:A:159:LEU:HD11	2.51	0.41
1:D:14:ARG:HB3	4:D:2008:HOH:O	2.21	0.40
1:C:231:GLU:OE1	1:C:231:GLU:N	2.41	0.40
1:C:65:ASN:HA	1:C:69:LEU:HD22	2.03	0.40
1:B:208:LEU:O	4:B:2009:HOH:O	2.22	0.40
1:D:13:LYS:HA	1:D:17:ARG:HD2	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:2019:HOH:O	4:C:2020:HOH:O[1_454]	1.97	0.23

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	245/288 (85%)	230 (94%)	14 (6%)	1 (0%)	39	42
1	B	246/288 (85%)	230 (94%)	16 (6%)	0	100	100
1	C	245/288 (85%)	230 (94%)	15 (6%)	0	100	100
1	D	243/288 (84%)	230 (95%)	11 (4%)	2 (1%)	24	22
All	All	979/1152 (85%)	920 (94%)	56 (6%)	3 (0%)	46	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	208	LEU
1	A	223	ARG
1	D	14	ARG

5.3.2 Protein sidechains [i](#)

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	199/231 (86%)	194 (98%)	5 (2%)	55	67
1	B	200/231 (87%)	193 (96%)	7 (4%)	43	53
1	C	199/231 (86%)	197 (99%)	2 (1%)	82	91
1	D	197/231 (85%)	192 (98%)	5 (2%)	55	67
All	All	795/924 (86%)	776 (98%)	19 (2%)	57	69

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	44	LEU
1	A	151	SER
1	A	166	GLN
1	A	250	GLN
1	B	79	SER
1	B	95	SER
1	B	104	GLN
1	B	152	SER
1	B	159	LEU
1	B	179	HIS
1	B	250	GLN
1	C	235	GLU
1	C	242	ILE
1	D	4	PRO
1	D	44	LEU
1	D	159	LEU
1	D	208	LEU
1	D	213	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	GLN
1	A	250	GLN
1	B	140	GLN
1	B	250	GLN
1	C	175	ASN
1	C	186	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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	1269	-	42,52,52	0.99	2 (4%)	54,80,80	2.25	13 (24%)
3	UIH	A	1270	-	26,27,27	1.69	4 (15%)	27,39,39	1.69	4 (14%)
2	NAP	B	1269	-	42,52,52	0.94	2 (4%)	54,80,80	2.46	13 (24%)
3	UIH	B	1270	-	26,27,27	1.72	5 (19%)	27,39,39	1.78	5 (18%)
2	NAP	C	1269	-	42,52,52	0.89	2 (4%)	54,80,80	1.98	16 (29%)
3	UIH	C	1270	-	26,27,27	1.55	5 (19%)	27,39,39	1.54	2 (7%)
2	NAP	D	1269	-	42,52,52	1.18	4 (9%)	54,80,80	2.33	14 (25%)
3	UIH	D	1270	-	26,27,27	1.85	5 (19%)	27,39,39	1.36	3 (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	1269	-	-	0/27/67/67	0/5/5/5
3	UIH	A	1270	-	-	0/8/8/8	0/4/4/4
2	NAP	B	1269	-	-	0/27/67/67	0/5/5/5
3	UIH	B	1270	-	-	0/8/8/8	0/4/4/4
2	NAP	C	1269	-	-	0/27/67/67	0/5/5/5
3	UIH	C	1270	-	-	0/8/8/8	0/4/4/4
2	NAP	D	1269	-	-	0/27/67/67	0/5/5/5
3	UIH	D	1270	-	-	0/8/8/8	0/4/4/4

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1270	UIH	CAV-C5	-5.43	1.35	1.42
3	A	1270	UIH	CAV-C5	-4.72	1.36	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1270	UIH	CAV-C5	-4.22	1.36	1.42
3	B	1270	UIH	CAV-CAU	-3.63	1.37	1.41
3	B	1270	UIH	CAV-C5	-3.63	1.37	1.42
3	D	1270	UIH	CAV-CAU	-3.16	1.38	1.41
2	B	1269	NAP	O7N-C7N	-2.71	1.18	1.24
3	A	1270	UIH	CAV-CAU	-2.62	1.38	1.41
2	D	1269	NAP	C3N-C7N	-2.57	1.46	1.50
2	D	1269	NAP	O7N-C7N	-2.07	1.19	1.24
2	C	1269	NAP	C2A-N3A	2.00	1.35	1.32
3	C	1270	UIH	C6-NAB	2.01	1.41	1.34
2	D	1269	NAP	C5A-C4A	2.26	1.45	1.40
3	C	1270	UIH	CAV-CAT	2.39	1.52	1.49
3	D	1270	UIH	BR-CAP	2.44	1.95	1.90
3	A	1270	UIH	C6-NAB	2.52	1.42	1.34
3	C	1270	UIH	CAS-CAU	2.53	1.51	1.49
3	B	1270	UIH	C6-NAB	2.83	1.43	1.34
2	A	1269	NAP	O4B-C1B	2.92	1.44	1.41
2	B	1269	NAP	C5A-C4A	2.95	1.47	1.40
3	B	1270	UIH	BR-CAP	3.03	1.97	1.90
2	A	1269	NAP	C5A-C4A	3.13	1.47	1.40
2	C	1269	NAP	C5A-C4A	3.19	1.47	1.40
3	C	1270	UIH	C2-NAA	3.21	1.40	1.34
3	D	1270	UIH	C6-NAB	3.25	1.45	1.34
3	B	1270	UIH	C2-NAA	3.84	1.41	1.34
3	D	1270	UIH	C2-NAA	4.22	1.42	1.34
3	A	1270	UIH	C2-NAA	4.32	1.42	1.34
2	D	1269	NAP	O4B-C1B	4.67	1.47	1.41

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1269	NAP	N3A-C2A-N1A	-10.82	120.61	128.89
2	D	1269	NAP	N3A-C2A-N1A	-8.22	122.60	128.89
2	C	1269	NAP	N3A-C2A-N1A	-7.24	123.35	128.89
2	D	1269	NAP	C4B-O4B-C1B	-6.29	102.81	109.72
3	A	1270	UIH	N3-C2-N1	-6.02	118.27	127.44
3	B	1270	UIH	N3-C2-N1	-5.56	118.98	127.44
2	A	1269	NAP	N3A-C2A-N1A	-5.42	124.75	128.89
2	D	1269	NAP	C4A-C5A-N7A	-5.29	104.61	109.48
2	A	1269	NAP	C4B-O4B-C1B	-5.16	104.05	109.72
3	C	1270	UIH	N3-C2-N1	-5.11	119.66	127.44
3	D	1270	UIH	N3-C2-N1	-5.08	119.70	127.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1269	NAP	O7N-C7N-C3N	-4.90	114.23	119.59
2	A	1269	NAP	PN-O3-PA	-4.30	120.65	132.73
2	A	1269	NAP	C4A-C5A-N7A	-4.22	105.60	109.48
2	C	1269	NAP	C4B-O4B-C1B	-4.18	105.12	109.72
2	A	1269	NAP	O3-PA-O5B	-4.10	92.05	102.94
3	C	1270	UIH	CAT-CAV-CAU	-3.83	119.28	126.88
2	B	1269	NAP	PN-O3-PA	-3.62	122.57	132.73
2	C	1269	NAP	O7N-C7N-N7N	-3.62	117.50	122.59
2	C	1269	NAP	C4A-C5A-N7A	-3.57	106.20	109.48
2	B	1269	NAP	O2B-P2B-O1X	-3.53	98.28	107.11
2	C	1269	NAP	C1B-N9A-C4A	-3.51	121.64	126.94
3	A	1270	UIH	CAT-CAV-CAU	-3.38	120.18	126.88
2	B	1269	NAP	C4D-O4D-C1D	-3.33	106.06	109.72
2	B	1269	NAP	C4A-C5A-N7A	-3.33	106.42	109.48
2	B	1269	NAP	C1B-N9A-C4A	-3.20	122.11	126.94
2	D	1269	NAP	C1B-N9A-C4A	-3.05	122.34	126.94
2	B	1269	NAP	C4B-O4B-C1B	-3.03	106.39	109.72
3	B	1270	UIH	CAI-CAT-CAV	-3.01	116.06	120.76
2	D	1269	NAP	PN-O3-PA	-3.00	124.31	132.73
2	D	1269	NAP	O3-PA-O5B	-2.99	95.02	102.94
2	C	1269	NAP	PN-O3-PA	-2.60	125.43	132.73
2	D	1269	NAP	O2B-P2B-O1X	-2.57	100.70	107.11
3	A	1270	UIH	CAV-C5-C4	-2.53	105.52	107.54
3	B	1270	UIH	CAT-CAV-CAU	-2.51	121.90	126.88
3	D	1270	UIH	CAK-CAS-CAU	-2.47	116.74	120.60
2	A	1269	NAP	C1B-N9A-C4A	-2.35	123.40	126.94
2	C	1269	NAP	O5B-PA-O1A	-2.30	100.70	109.62
2	A	1269	NAP	O2B-P2B-O1X	-2.12	101.82	107.11
2	A	1269	NAP	O7N-C7N-C3N	-2.06	117.34	119.59
2	D	1269	NAP	O7N-C7N-C3N	-2.06	117.34	119.59
2	C	1269	NAP	C2N-C3N-C4N	-2.01	116.05	118.29
2	D	1269	NAP	O3-PN-O5D	2.02	108.30	102.94
2	C	1269	NAP	O7N-C7N-C3N	2.13	121.91	119.59
2	D	1269	NAP	C2N-C3N-C4N	2.14	120.67	118.29
2	B	1269	NAP	O4D-C4D-C3D	2.19	109.56	105.15
2	C	1269	NAP	O4B-C1B-N9A	2.25	112.80	108.10
2	C	1269	NAP	C2A-N1A-C6A	2.26	122.81	118.77
2	A	1269	NAP	O3X-P2B-O2X	2.30	116.15	107.38
2	C	1269	NAP	O2N-PN-O1N	2.32	125.10	112.53
2	A	1269	NAP	C2A-N1A-C6A	2.42	123.10	118.77
3	D	1270	UIH	NAA-C2-N1	2.43	121.22	117.20
2	C	1269	NAP	C3N-C7N-N7N	2.50	120.55	117.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1270	UIH	CAJ-CAT-CAV	2.76	125.08	120.76
2	C	1269	NAP	O4D-C1D-N1N	2.94	111.36	108.13
3	A	1270	UIH	NAA-C2-N1	3.10	122.33	117.20
2	D	1269	NAP	O2A-PA-O3	3.12	119.26	105.09
2	B	1269	NAP	C2A-N1A-C6A	3.15	124.39	118.77
2	C	1269	NAP	O3X-P2B-O2X	3.22	119.64	107.38
2	C	1269	NAP	P2B-O2B-C2B	3.23	129.31	121.56
2	B	1269	NAP	O4D-C1D-N1N	3.26	111.71	108.13
2	D	1269	NAP	C3N-C7N-N7N	3.45	121.59	117.82
2	A	1269	NAP	C3N-C7N-N7N	3.48	121.62	117.82
2	B	1269	NAP	O4B-C1B-N9A	3.60	115.62	108.10
3	B	1270	UIH	NAA-C2-N1	4.01	123.84	117.20
2	D	1269	NAP	O4B-C1B-N9A	4.42	117.35	108.10
2	A	1269	NAP	O4B-C1B-N9A	5.18	118.95	108.10
2	D	1269	NAP	O4D-C1D-N1N	6.52	115.30	108.13
2	B	1269	NAP	C3N-C7N-N7N	6.83	125.29	117.82
2	A	1269	NAP	O4D-C1D-N1N	7.76	116.66	108.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1269	NAP	1	0
3	A	1270	UIH	5	0
2	B	1269	NAP	1	0
3	B	1270	UIH	3	0
2	C	1269	NAP	1	0
3	C	1270	UIH	6	0
2	D	1269	NAP	1	0
3	D	1270	UIH	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	251/288 (87%)	-0.15	5 (1%) 68 67	6, 14, 30, 54	0
1	B	251/288 (87%)	-0.15	5 (1%) 68 67	6, 14, 29, 48	0
1	C	251/288 (87%)	-0.02	7 (2%) 56 55	8, 15, 38, 54	0
1	D	249/288 (86%)	-0.06	9 (3%) 46 45	7, 15, 38, 73	0
All	All	1002/1152 (86%)	-0.10	26 (2%) 59 58	6, 15, 34, 73	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	105	GLY	6.1
1	D	212	ALA	5.7
1	D	211	VAL	5.3
1	C	211	VAL	4.9
1	B	113	GLY	4.4
1	A	151	SER	4.0
1	A	104	GLN	3.7
1	C	212	ALA	3.7
1	C	151	SER	3.5
1	C	104	GLN	3.4
1	B	104	GLN	3.2
1	D	113	GLY	3.1
1	B	152	SER	3.1
1	A	113	GLY	3.0
1	D	152	SER	3.0
1	B	211	VAL	2.8
1	D	218	LYS	2.6
1	D	210	PRO	2.6
1	D	216	GLU	2.6
1	C	152	SER	2.6
1	A	152	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	2	GLU	2.4
1	C	2	GLU	2.3
1	D	213	MET	2.2
1	B	54	ASN	2.1
1	A	212	ALA	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	UIH	C	1270	24/24	0.95	0.14	0.91	18,26,31,33	0
3	UIH	B	1270	24/24	0.95	0.14	0.39	14,17,20,23	0
3	UIH	D	1270	24/24	0.95	0.13	-0.19	16,21,24,27	0
2	NAP	A	1269	48/48	0.96	0.10	-0.71	7,9,13,13	0
3	UIH	A	1270	24/24	0.97	0.10	-0.72	15,20,22,25	0
2	NAP	C	1269	48/48	0.96	0.09	-1.11	9,12,14,15	0
2	NAP	D	1269	48/48	0.96	0.09	-1.13	10,13,17,18	0
2	NAP	B	1269	48/48	0.97	0.10	-1.26	5,9,11,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.