Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:02 AM GMT

PDB ID	:	3KJS
Title	:	Crystal Structure of T. cruzi DHFR-TS with 3 high affinity DHFR inhibitors: DQ1 inhibitor complex
Authors	:	Schormann, N.; Senkovich, O.; Chattopadhyay, D.
Deposited on	:	2009-11-03
Resolution	:	2.50 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

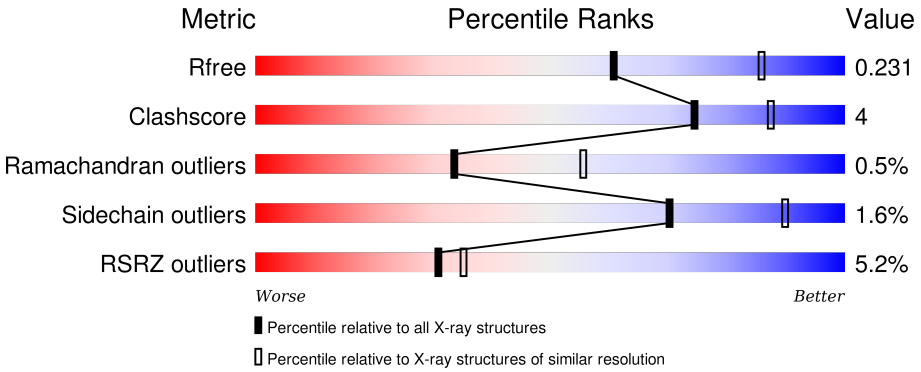
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	521	6% 87% 8% ·
1	B	521	6% 87% 8% · ·
1	C	521	5% 87% 9% · ·
1	D	521	3% 88% 8% ·

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
2	DQ1	C	602	-	-	-	X
5	EDO	A	906	-	-	-	X
5	EDO	B	905	-	-	-	X
5	EDO	D	908	-	-	X	X

2 Entry composition

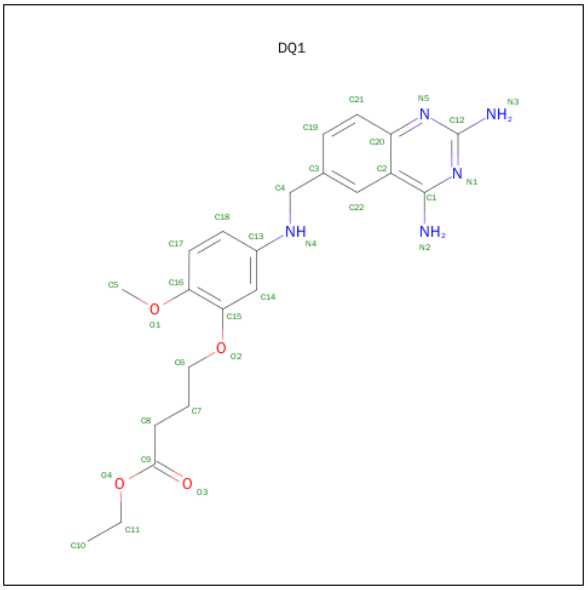
There are 6 unique types of molecules in this entry. The entry contains 17053 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dihydrofolate reductase-thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	500	Total	C	N	O	S	0	0	0
			3950	2512	695	725	18			
1	B	499	Total	C	N	O	S	0	0	0
			3956	2515	696	727	18			
1	C	507	Total	C	N	O	S	0	1	0
			4011	2546	707	739	19			
1	D	504	Total	C	N	O	S	0	0	0
			3991	2535	704	734	18			

- Molecule 2 is ETHYL 4-(5-{[(2,4-DIAMINOQUINAZOLIN-6-YL)METHYL]AMINO}-2-METHOXYPHENOXY)BUTANOATE (three-letter code: DQ1) (formula: $C_{22}H_{27}N_5O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			31	22	5	4		
2	B	1	Total	C	N	O	0	0
			31	22	5	4		

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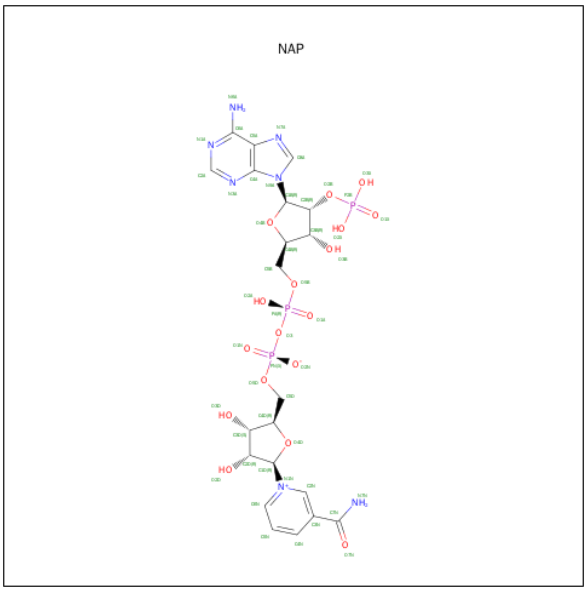
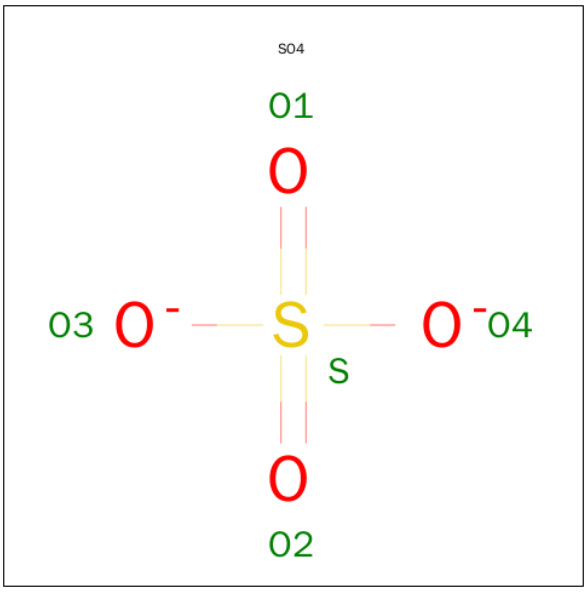
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C N O 31 22 5 4	0	0
2	D	1	Total C N O 31 22 5 4	0	0

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



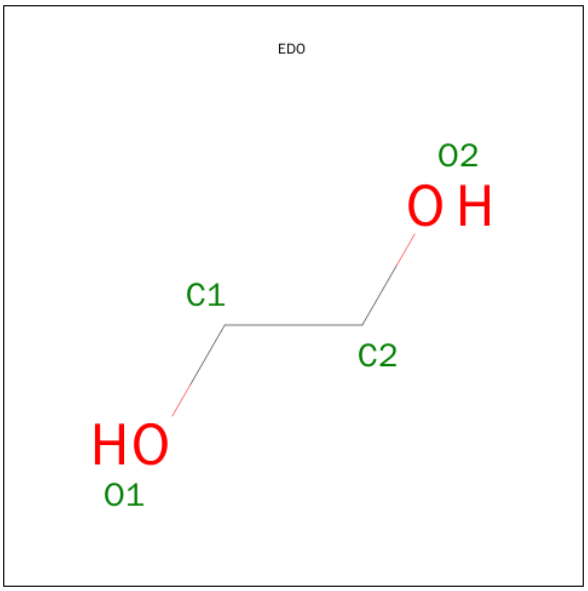
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 48 21 7 17 3	0	0
3	B	1	Total C N O P 48 21 7 17 3	0	0
3	C	1	Total C N O P 48 21 7 17 3	0	0
3	D	1	Total C N O P 48 21 7 17 3	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0

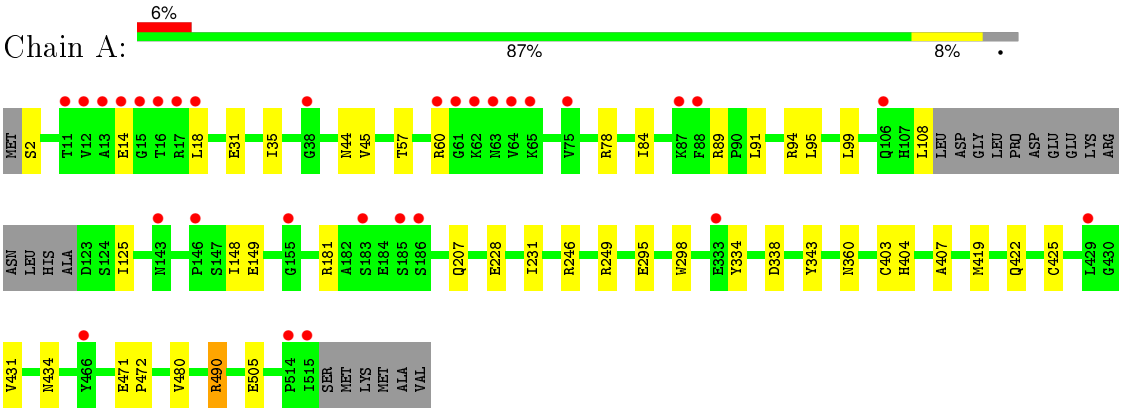
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	157	Total O 157 157	0	0
6	B	168	Total O 168 168	0	0
6	C	204	Total O 204 204	0	0
6	D	208	Total O 208 208	0	0

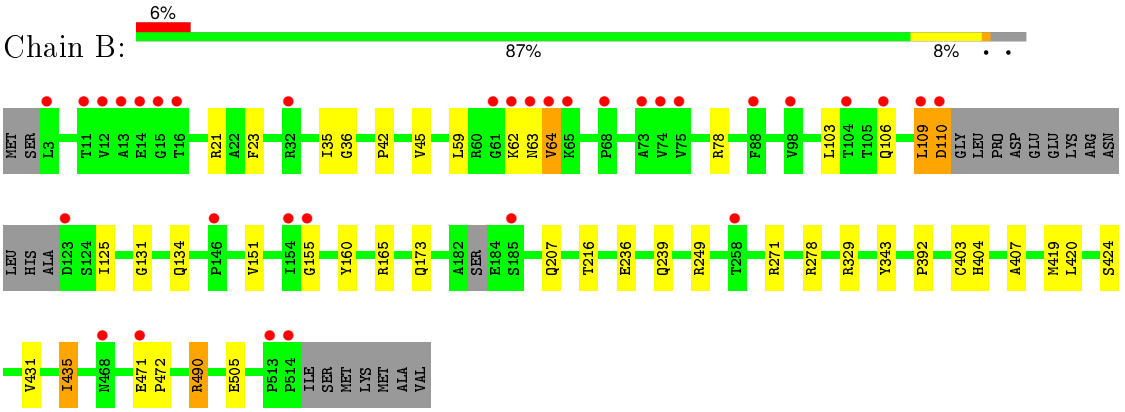
3 Residue-property plots (i)

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.

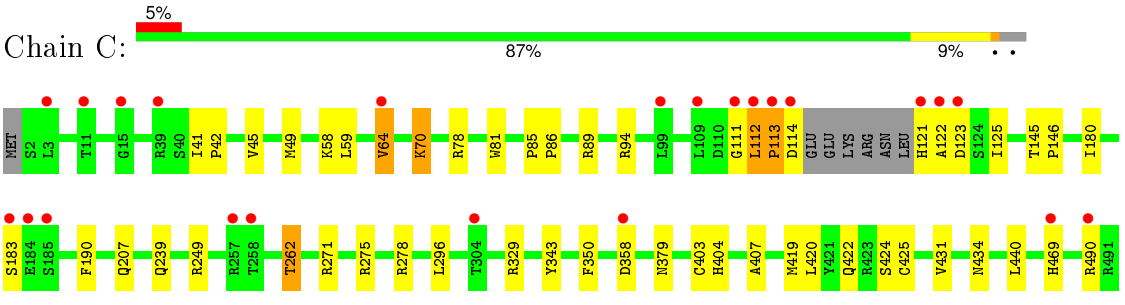
- Molecule 1: Dihydrofolate reductase-thymidylate synthase

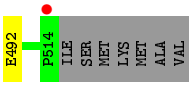


- Molecule 1: Dihydrofolate reductase-thymidylate synthase



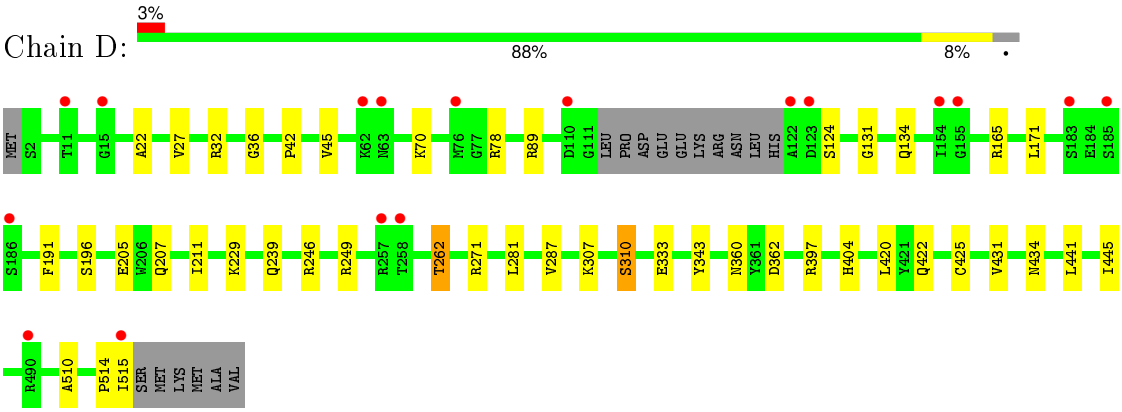
- Molecule 1: Dihydrofolate reductase-thymidylate synthase





• Molecule 1: Dihydrofolate reductase-thymidylate synthase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	175.62Å 175.62Å 249.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 19.99 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-2.50) 99.6 (19.99-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	3.42 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.200 , 0.234 0.201 , 0.231	Depositor DCC
R_{free} test set	6726 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	42.9	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 39.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	2 of 133693 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	17053	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.14% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, DQ1, EDO, SO4

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	0.39	0/4045	0.53	0/5492
1	B	0.39	0/4050	0.54	0/5496
1	C	0.39	0/4110	0.54	0/5579
1	D	0.38	0/4086	0.53	0/5545
All	All	0.39	0/16291	0.54	0/22112

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	3950	0	3896	30	0
1	B	3956	0	3906	29	0
1	C	4011	0	3956	42	0
1	D	3991	0	3947	36	0
2	A	31	0	27	4	0
2	B	31	0	27	2	0
2	C	31	0	27	7	0
2	D	31	0	27	4	0
3	A	48	0	25	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	48	0	25	1	0
3	C	48	0	25	1	0
3	D	48	0	25	1	0
4	A	5	0	0	0	0
4	B	10	0	0	0	0
4	C	10	0	0	0	0
4	D	15	0	0	0	0
5	A	16	0	24	0	0
5	B	12	0	18	0	0
5	C	8	0	12	0	0
5	D	16	0	24	6	0
6	A	157	0	0	4	0
6	B	168	0	0	1	0
6	C	204	0	0	3	0
6	D	208	0	0	2	0
All	All	17053	0	15991	130	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 4.

All (130) 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:C:45:VAL:H	2:C:602:DQ1:H10A	1.37	0.88
1:C:49:MET:HE2	2:C:602:DQ1:H21	1.59	0.85
1:A:60:ARG:HG3	1:A:149:GLU:OE2	1.78	0.84
1:C:49:MET:CE	2:C:602:DQ1:H21	2.10	0.82
1:D:45:VAL:H	2:D:602:DQ1:H10A	1.47	0.78
1:B:471:GLU:HB3	1:B:472:PRO:HD3	1.70	0.73
1:C:112:LEU:CB	1:C:113:PRO:HA	2.20	0.70
1:B:106:GLN:HA	1:B:109:LEU:HD12	1.75	0.69
1:C:404:HIS:HB2	1:C:420:LEU:HD11	1.74	0.69
1:A:231:ILE:HD11	1:A:480:VAL:HG11	1.75	0.68
1:B:404:HIS:HB2	1:B:420:LEU:HD11	1.77	0.67
1:A:2:SER:HB3	6:A:524:HOH:O	1.93	0.66
1:C:121:HIS:O	1:C:123:ASP:N	2.30	0.65
1:D:78:ARG:HD3	3:D:702:NAP:O2X	1.97	0.64
1:C:113:PRO:O	1:C:114:ASP:CB	2.45	0.63
1:B:59:LEU:H	1:B:64:VAL:HG13	1.64	0.63
1:D:131:GLY:H	1:D:134:GLN:HE21	1.46	0.63
1:C:45:VAL:H	2:C:602:DQ1:C10	2.11	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:GLN:HE22	1:C:271:ARG:H	1.48	0.60
1:D:514:PRO:O	1:D:515:ILE:HB	2.02	0.59
1:B:59:LEU:H	1:B:64:VAL:CG1	2.15	0.59
1:B:109:LEU:C	1:B:110:ASP:OD1	2.41	0.58
1:C:113:PRO:O	1:C:114:ASP:HB2	2.02	0.58
1:C:112:LEU:H	1:C:113:PRO:HA	1.68	0.58
1:B:236:GLU:OE1	1:B:278:ARG:NH2	2.37	0.58
1:C:112:LEU:CB	1:C:113:PRO:CA	2.82	0.57
6:A:525:HOH:O	1:D:262:THR:HG21	2.04	0.56
1:C:59:LEU:H	1:C:64:VAL:HG13	1.70	0.56
1:D:404:HIS:HB2	1:D:420:LEU:HD11	1.87	0.56
1:C:49:MET:HE1	2:C:602:DQ1:H21	1.88	0.55
1:A:471:GLU:HB3	1:A:472:PRO:HD3	1.88	0.55
1:B:36:GLY:HA2	1:B:42:PRO:HD3	1.88	0.55
1:C:403[B]:CYS:SG	1:C:424:SER:O	2.65	0.54
1:C:78:ARG:HD3	3:C:702:NAP:O2X	2.07	0.54
1:C:207:GLN:NE2	1:D:249:ARG:HH11	2.04	0.54
1:A:78:ARG:HD3	3:A:702:NAP:O2X	2.07	0.54
1:D:36:GLY:HA2	1:D:42:PRO:HD3	1.90	0.54
1:D:45:VAL:H	2:D:602:DQ1:C10	2.18	0.53
1:A:14:GLU:OE1	1:C:190:PHE:CZ	2.61	0.53
1:A:31:GLU:OE2	1:A:181:ARG:HD2	2.07	0.53
1:A:95:LEU:HD22	1:A:148:ILE:HD11	1.90	0.53
1:A:108:LEU:HD12	1:A:125:ILE:HD12	1.90	0.53
1:A:45:VAL:H	2:A:602:DQ1:H10A	1.74	0.52
1:A:246:ARG:NH2	6:A:575:HOH:O	2.43	0.52
1:D:229:LYS:HZ1	5:D:908:EDO:H11	1.75	0.52
1:A:91:LEU:HB3	1:A:94:ARG:HH21	1.75	0.52
1:A:84:ILE:O	1:A:89:ARG:NH1	2.37	0.51
1:C:207:GLN:HE22	1:D:249:ARG:HH11	1.56	0.51
1:B:490:ARG:HD2	1:B:505:GLU:OE1	2.10	0.51
1:B:109:LEU:O	1:B:110:ASP:OD1	2.30	0.50
1:C:407:ALA:HA	1:C:419:MET:O	2.11	0.50
1:D:510:ALA:HB1	5:D:908:EDO:H12	1.94	0.49
1:C:422:GLN:HE22	1:C:434:ASN:HD22	1.59	0.49
1:A:334:TYR:HB3	1:A:338:ASP:HB3	1.93	0.49
1:B:431:VAL:O	1:B:435:ILE:HG12	2.12	0.49
1:C:379:ASN:ND2	6:C:556:HOH:O	2.44	0.49
1:A:425:CYS:HB3	1:A:431:VAL:CG2	2.42	0.49
1:B:165:ARG:NH2	1:D:165:ARG:HE	2.10	0.49
1:C:58:LYS:HA	1:C:64:VAL:HG11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:ALA:HA	1:B:419:MET:O	2.13	0.48
1:B:59:LEU:HB2	1:B:64:VAL:HG13	1.94	0.48
1:D:422:GLN:HE22	1:D:434:ASN:ND2	2.11	0.48
2:C:602:DQ1:H14	2:C:602:DQ1:H6	1.66	0.48
6:B:572:HOH:O	1:C:262:THR:HG21	2.13	0.48
1:B:165:ARG:HH21	1:D:165:ARG:HE	1.62	0.48
1:D:360:ASN:HD21	1:D:362:ASP:HB2	1.79	0.48
1:D:211:ILE:HD11	5:D:903:EDO:H12	1.96	0.47
1:A:422:GLN:HE22	1:A:434:ASN:ND2	2.13	0.47
1:D:239:GLN:HE22	1:D:271:ARG:H	1.62	0.47
1:A:44:ASN:HA	2:A:602:DQ1:H10A	1.97	0.47
1:C:249:ARG:HD2	1:D:207:GLN:NE2	2.30	0.47
1:D:441:LEU:O	1:D:445:ILE:HG12	2.14	0.46
1:D:425:CYS:HB3	1:D:431:VAL:CG2	2.45	0.46
1:D:422:GLN:HE22	1:D:434:ASN:HD22	1.64	0.46
1:D:333:GLU:OE2	1:D:397:ARG:NH2	2.32	0.46
1:D:246:ARG:NH2	6:D:588:HOH:O	2.50	0.45
1:C:249:ARG:HH11	1:D:207:GLN:NE2	2.13	0.45
1:D:27:VAL:HG11	1:D:191:PHE:CE2	2.52	0.45
1:B:131:GLY:N	1:B:134:GLN:HE21	2.15	0.45
1:A:249:ARG:NH1	1:B:207:GLN:OE1	2.49	0.45
1:C:275:ARG:O	1:C:278:ARG:HD2	2.17	0.44
1:A:490:ARG:HD2	1:A:505:GLU:OE1	2.17	0.44
1:D:229:LYS:NZ	5:D:908:EDO:H11	2.32	0.44
1:B:23:PHE:O	1:B:173:GLN:HG2	2.18	0.44
1:A:45:VAL:H	2:A:602:DQ1:C10	2.31	0.44
1:B:35:ILE:O	3:B:702:NAP:H2N	2.18	0.44
1:A:99:LEU:O	3:A:702:NAP:H1B	2.18	0.44
1:A:228:GLU:HG2	6:A:522:HOH:O	2.17	0.44
1:B:131:GLY:H	1:B:134:GLN:HE21	1.65	0.44
1:D:131:GLY:N	1:D:134:GLN:HE21	2.15	0.44
1:B:392:PRO:HD2	1:C:350:PHE:CZ	2.53	0.44
2:B:602:DQ1:H14	2:B:602:DQ1:H6	1.62	0.44
1:B:239:GLN:HE22	1:B:271:ARG:H	1.66	0.43
1:D:249:ARG:NH2	6:D:590:HOH:O	2.51	0.43
1:A:57:THR:OG1	1:A:94:ARG:NH1	2.51	0.43
2:D:602:DQ1:H14	2:D:602:DQ1:H6	1.62	0.43
1:B:403:CYS:SG	1:B:424:SER:O	2.77	0.43
1:C:422:GLN:HE22	1:C:434:ASN:ND2	2.16	0.43
1:C:145:THR:HA	1:C:146:PRO:HA	1.88	0.43
1:B:78:ARG:HG3	1:B:103:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:LEU:HB3	1:A:94:ARG:NH2	2.33	0.43
1:D:211:ILE:CD1	5:D:903:EDO:H12	2.49	0.43
1:A:407:ALA:HA	1:A:419:MET:O	2.19	0.43
1:C:425:CYS:HB3	1:C:431:VAL:CG2	2.49	0.43
1:C:81:TRP:CH2	1:C:125:ILE:HD12	2.54	0.42
1:B:131:GLY:H	1:B:134:GLN:NE2	2.17	0.42
1:C:112:LEU:N	1:C:113:PRO:HA	2.25	0.42
1:A:207:GLN:OE1	1:B:249:ARG:HD2	2.19	0.42
1:D:22:ALA:HA	1:D:171:LEU:HB3	2.01	0.42
2:A:602:DQ1:H6	2:A:602:DQ1:H14	1.62	0.41
1:C:45:VAL:N	2:C:602:DQ1:H10A	2.20	0.41
1:A:35:ILE:O	3:A:702:NAP:H2N	2.20	0.41
1:D:307:LYS:HA	1:D:310:SER:HB2	2.02	0.41
1:A:295:GLU:O	1:A:298:TRP:HB3	2.20	0.41
1:D:281:LEU:HD22	1:D:287:VAL:HB	2.02	0.41
1:C:45:VAL:HG21	1:C:180:ILE:HD12	2.02	0.41
1:D:196:SER:OG	1:D:205:GLU:HG3	2.20	0.41
1:D:45:VAL:N	2:D:602:DQ1:H10A	2.25	0.41
1:B:21:ARG:HG2	1:B:151:VAL:HG21	2.02	0.41
1:A:404:HIS:CD2	1:A:404:HIS:H	2.39	0.41
1:D:510:ALA:CB	5:D:908:EDO:H12	2.50	0.41
1:C:70:LYS:HE2	6:C:637:HOH:O	2.21	0.41
1:A:14:GLU:OE1	1:C:190:PHE:CE2	2.74	0.41
1:B:155:GLY:HA2	1:B:160:TYR:CZ	2.56	0.41
1:C:85:PRO:HA	1:C:86:PRO:HD3	1.95	0.40
1:B:45:VAL:H	2:B:602:DQ1:H10A	1.85	0.40
1:C:111:GLY:O	6:C:546:HOH:O	2.22	0.40
1:C:41:ILE:HA	1:C:42:PRO:HD3	1.95	0.40
1:C:59:LEU:H	1:C:64:VAL:CG1	2.33	0.40
1:C:296:LEU:HD22	1:C:440:LEU:HG	2.04	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	496/521 (95%)	483 (97%)	12 (2%)	1 (0%)	52	75
1	B	493/521 (95%)	476 (97%)	14 (3%)	3 (1%)	30	50
1	C	504/521 (97%)	486 (96%)	13 (3%)	5 (1%)	19	34
1	D	500/521 (96%)	489 (98%)	10 (2%)	1 (0%)	52	75
All	All	1993/2084 (96%)	1934 (97%)	49 (2%)	10 (0%)	34	55

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	122	ALA
1	B	64	VAL
1	D	343	TYR
1	B	109	LEU
1	B	343	TYR
1	C	343	TYR
1	A	343	TYR
1	C	112	LEU
1	C	113	PRO
1	C	64	VAL

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	421/446 (94%)	417 (99%)	4 (1%)	82	95
1	B	423/446 (95%)	415 (98%)	8 (2%)	65	87
1	C	429/446 (96%)	419 (98%)	10 (2%)	58	83
1	D	427/446 (96%)	421 (99%)	6 (1%)	74	91
All	All	1700/1784 (95%)	1672 (98%)	28 (2%)	70	90

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	360	ASN
1	A	403	CYS
1	A	490	ARG
1	B	62	LYS
1	B	63	ASN
1	B	110	ASP
1	B	125	ILE
1	B	216	THR
1	B	329	ARG
1	B	435	ILE
1	B	490	ARG
1	C	70	LYS
1	C	89	ARG
1	C	94	ARG
1	C	183	SER
1	C	262	THR
1	C	329	ARG
1	C	358	ASP
1	C	469	HIS
1	C	490	ARG
1	C	492	GLU
1	D	32	ARG
1	D	70	LYS
1	D	89	ARG
1	D	124	SER
1	D	262	THR
1	D	310	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	GLN
1	A	239	GLN
1	A	315	HIS
1	A	360	ASN
1	A	434	ASN
1	A	469	HIS
1	B	134	GLN
1	B	239	GLN
1	B	315	HIS
1	B	320	ASN
1	B	422	GLN

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Mol	Chain	Res	Type
1	B	434	ASN
1	B	469	HIS
1	C	173	GLN
1	C	207	GLN
1	C	239	GLN
1	C	269	GLN
1	C	315	HIS
1	C	320	ASN
1	C	346	GLN
1	C	360	ASN
1	C	379	ASN
1	C	434	ASN
1	D	134	GLN
1	D	207	GLN
1	D	239	GLN
1	D	315	HIS
1	D	346	GLN
1	D	360	ASN
1	D	434	ASN
1	D	469	HIS

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

29 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	DQ1	A	602	-	33,33,33	1.49	1 (3%)	41,44,44	1.58	6 (14%)
4	SO4	A	701	-	4,4,4	0.18	0	6,6,6	0.13	0
3	NAP	A	702	-	42,52,52	1.25	6 (14%)	54,80,80	2.19	8 (14%)
5	EDO	A	901	-	3,3,3	0.51	0	2,2,2	0.44	0
5	EDO	A	902	-	3,3,3	0.42	0	2,2,2	0.57	0
5	EDO	A	906	-	3,3,3	0.50	0	2,2,2	0.28	0
5	EDO	A	907	-	3,3,3	0.46	0	2,2,2	0.46	0
4	SO4	B	601	-	4,4,4	0.28	0	6,6,6	0.25	0
2	DQ1	B	602	-	33,33,33	1.51	1 (3%)	41,44,44	1.60	7 (17%)
4	SO4	B	701	-	4,4,4	0.20	0	6,6,6	0.11	0
3	NAP	B	702	-	42,52,52	1.25	5 (11%)	54,80,80	2.11	9 (16%)
5	EDO	B	904	-	3,3,3	0.47	0	2,2,2	0.44	0
5	EDO	B	905	-	3,3,3	0.49	0	2,2,2	0.48	0
5	EDO	B	912	-	3,3,3	0.45	0	2,2,2	0.51	0
2	DQ1	C	602	-	33,33,33	1.56	1 (3%)	41,44,44	1.47	5 (12%)
4	SO4	C	701	-	4,4,4	0.19	0	6,6,6	0.10	0
3	NAP	C	702	-	42,52,52	1.27	5 (11%)	54,80,80	2.17	11 (20%)
4	SO4	C	801	-	4,4,4	0.29	0	6,6,6	0.16	0
5	EDO	C	909	-	3,3,3	0.44	0	2,2,2	0.39	0
5	EDO	C	913	-	3,3,3	0.47	0	2,2,2	0.40	0
4	SO4	D	522	-	4,4,4	0.19	0	6,6,6	0.24	0
4	SO4	D	601	-	4,4,4	0.28	0	6,6,6	0.28	0
2	DQ1	D	602	-	33,33,33	1.62	1 (3%)	41,44,44	1.68	6 (14%)
4	SO4	D	701	-	4,4,4	0.18	0	6,6,6	0.09	0
3	NAP	D	702	-	42,52,52	1.31	5 (11%)	54,80,80	2.21	9 (16%)
5	EDO	D	903	-	3,3,3	0.43	0	2,2,2	0.46	0
5	EDO	D	908	-	3,3,3	0.43	0	2,2,2	0.57	0
5	EDO	D	910	-	3,3,3	0.51	0	2,2,2	0.32	0
5	EDO	D	911	-	3,3,3	0.46	0	2,2,2	0.47	0

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	DQ1	A	602	-	-	0/17/17/17	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	A	701	-	-	0/0/0/0	0/0/0/0
3	NAP	A	702	-	-	0/27/67/67	0/5/5/5
5	EDO	A	901	-	-	0/1/1/1	0/0/0/0
5	EDO	A	902	-	-	0/1/1/1	0/0/0/0
5	EDO	A	906	-	-	0/1/1/1	0/0/0/0
5	EDO	A	907	-	-	0/1/1/1	0/0/0/0
4	SO4	B	601	-	-	0/0/0/0	0/0/0/0
2	DQ1	B	602	-	-	0/17/17/17	0/3/3/3
4	SO4	B	701	-	-	0/0/0/0	0/0/0/0
3	NAP	B	702	-	-	0/27/67/67	0/5/5/5
5	EDO	B	904	-	-	0/1/1/1	0/0/0/0
5	EDO	B	905	-	-	0/1/1/1	0/0/0/0
5	EDO	B	912	-	-	0/1/1/1	0/0/0/0
2	DQ1	C	602	-	-	0/17/17/17	0/3/3/3
4	SO4	C	701	-	-	0/0/0/0	0/0/0/0
3	NAP	C	702	-	-	0/27/67/67	0/5/5/5
4	SO4	C	801	-	-	0/0/0/0	0/0/0/0
5	EDO	C	909	-	-	0/1/1/1	0/0/0/0
5	EDO	C	913	-	-	0/1/1/1	0/0/0/0
4	SO4	D	522	-	-	0/0/0/0	0/0/0/0
4	SO4	D	601	-	-	0/0/0/0	0/0/0/0
2	DQ1	D	602	-	-	0/17/17/17	0/3/3/3
4	SO4	D	701	-	-	0/0/0/0	0/0/0/0
3	NAP	D	702	-	-	0/27/67/67	0/5/5/5
5	EDO	D	903	-	-	0/1/1/1	0/0/0/0
5	EDO	D	908	-	-	0/1/1/1	0/0/0/0
5	EDO	D	910	-	-	0/1/1/1	0/0/0/0
5	EDO	D	911	-	-	0/1/1/1	0/0/0/0

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	602	DQ1	C1-C2	-7.87	1.39	1.45
2	C	602	DQ1	C1-C2	-7.44	1.40	1.45
2	B	602	DQ1	C1-C2	-7.13	1.40	1.45
2	A	602	DQ1	C1-C2	-6.87	1.40	1.45
3	A	702	NAP	C6N-N1N	2.04	1.40	1.35
3	D	702	NAP	C3N-C7N	2.04	1.53	1.50
3	A	702	NAP	P2B-O2X	2.07	1.62	1.54
3	B	702	NAP	PA-O2A	2.09	1.63	1.54
3	C	702	NAP	C6N-N1N	2.12	1.41	1.35
3	D	702	NAP	C6N-N1N	2.16	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	NAP	C3N-C7N	2.18	1.54	1.50
3	D	702	NAP	P2B-O2X	2.22	1.62	1.54
3	C	702	NAP	P2B-O3X	2.30	1.63	1.54
3	C	702	NAP	P2B-O2X	2.31	1.63	1.54
3	A	702	NAP	C3N-C7N	2.37	1.54	1.50
3	A	702	NAP	P2B-O3X	2.38	1.63	1.54
3	B	702	NAP	C6N-N1N	2.45	1.42	1.35
3	B	702	NAP	O4D-C1D	2.66	1.44	1.41
3	A	702	NAP	O4D-C1D	2.76	1.44	1.41
3	C	702	NAP	O4D-C1D	2.93	1.44	1.41
3	D	702	NAP	O4D-C1D	2.98	1.45	1.41
3	A	702	NAP	O4B-C1B	4.36	1.46	1.41
3	B	702	NAP	O4B-C1B	4.66	1.47	1.41
3	C	702	NAP	O4B-C1B	4.89	1.47	1.41
3	D	702	NAP	O4B-C1B	5.24	1.47	1.41

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	702	NAP	N3A-C2A-N1A	-10.09	121.17	128.89
3	B	702	NAP	N3A-C2A-N1A	-9.79	121.40	128.89
3	D	702	NAP	N3A-C2A-N1A	-9.74	121.44	128.89
3	C	702	NAP	N3A-C2A-N1A	-9.70	121.47	128.89
3	A	702	NAP	O3-PN-O5D	-8.77	79.67	102.94
3	D	702	NAP	O3-PN-O5D	-8.66	79.97	102.94
3	C	702	NAP	O3-PN-O5D	-8.66	79.97	102.94
3	B	702	NAP	O3-PN-O5D	-7.37	83.39	102.94
2	B	602	DQ1	N5-C12-N1	-4.62	120.40	127.44
2	A	602	DQ1	N5-C12-N1	-4.60	120.44	127.44
2	C	602	DQ1	N5-C12-N1	-4.48	120.62	127.44
2	D	602	DQ1	N5-C12-N1	-4.40	120.74	127.44
2	D	602	DQ1	C22-C2-C1	-4.20	121.32	124.74
3	D	702	NAP	C4D-O4D-C1D	-3.73	105.62	109.72
3	D	702	NAP	O2N-PN-O3	-3.43	89.53	105.09
3	A	702	NAP	O2N-PN-O3	-3.30	90.10	105.09
3	C	702	NAP	C4D-O4D-C1D	-3.28	106.12	109.72
2	A	602	DQ1	C2-C20-N5	-3.26	119.71	122.90
2	B	602	DQ1	C2-C20-N5	-3.26	119.72	122.90
2	C	602	DQ1	C22-C2-C1	-3.26	122.09	124.74
2	B	602	DQ1	C22-C2-C1	-3.25	122.10	124.74
3	B	702	NAP	C4D-O4D-C1D	-3.24	106.16	109.72
2	A	602	DQ1	C22-C2-C1	-3.22	122.12	124.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	702	NAP	O2N-PN-O3	-3.12	90.93	105.09
2	D	602	DQ1	C2-C20-N5	-3.09	119.89	122.90
3	A	702	NAP	C4D-O4D-C1D	-3.04	106.38	109.72
3	C	702	NAP	O2N-PN-O3	-2.87	92.06	105.09
2	C	602	DQ1	C2-C20-N5	-2.78	120.18	122.90
3	D	702	NAP	C4A-C5A-N7A	-2.40	107.27	109.48
3	B	702	NAP	C5D-C4D-C3D	-2.34	105.91	115.21
3	C	702	NAP	C4A-C5A-N7A	-2.31	107.36	109.48
3	D	702	NAP	C3N-C7N-N7N	-2.24	115.36	117.82
3	C	702	NAP	C3N-C7N-N7N	-2.20	115.41	117.82
3	B	702	NAP	C4A-C5A-N7A	-2.17	107.48	109.48
2	B	602	DQ1	O1-C16-C17	-2.14	120.75	124.35
3	B	702	NAP	PN-O3-PA	-2.13	126.75	132.73
3	A	702	NAP	C4A-C5A-N7A	-2.12	107.53	109.48
3	A	702	NAP	C3N-C7N-N7N	-2.06	115.56	117.82
3	C	702	NAP	C5D-C4D-C3D	-2.05	107.07	115.21
3	A	702	NAP	O2N-PN-O5D	2.10	119.06	108.46
3	C	702	NAP	O2B-P2B-O1X	2.12	112.39	107.11
2	C	602	DQ1	O4-C9-C8	2.17	118.51	111.90
3	C	702	NAP	O5D-PN-O1N	2.17	118.05	109.62
3	D	702	NAP	O2B-P2B-O1X	2.19	112.57	107.11
2	A	602	DQ1	O1-C16-C15	2.22	118.57	115.40
3	D	702	NAP	O2N-PN-O5D	2.23	119.72	108.46
3	B	702	NAP	O5D-PN-O1N	2.27	118.44	109.62
2	D	602	DQ1	O4-C9-C8	2.30	118.90	111.90
3	C	702	NAP	O4D-C1D-N1N	2.32	110.68	108.13
2	A	602	DQ1	O4-C9-C8	2.40	119.22	111.90
2	D	602	DQ1	O1-C16-C15	2.43	118.87	115.40
2	B	602	DQ1	O4-C9-C8	2.45	119.36	111.90
3	C	702	NAP	O4B-C1B-N9A	2.71	113.78	108.10
2	B	602	DQ1	O1-C16-C15	2.92	119.56	115.40
3	A	702	NAP	O4B-C1B-N9A	2.93	114.23	108.10
3	B	702	NAP	O4B-C1B-N9A	3.04	114.46	108.10
3	D	702	NAP	O4B-C1B-N9A	3.17	114.74	108.10
2	B	602	DQ1	C1-C2-C20	3.96	118.15	115.78
2	C	602	DQ1	C1-C2-C20	4.06	118.20	115.78
2	A	602	DQ1	C1-C2-C20	4.23	118.30	115.78
2	D	602	DQ1	C1-C2-C20	4.76	118.62	115.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	602	DQ1	4	0
3	A	702	NAP	3	0
2	B	602	DQ1	2	0
3	B	702	NAP	1	0
2	C	602	DQ1	7	0
3	C	702	NAP	1	0
2	D	602	DQ1	4	0
3	D	702	NAP	1	0
5	D	903	EDO	2	0
5	D	908	EDO	4	0

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, 95^{th} 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	500/521 (95%)	0.05	30 (6%)	25	28	26, 42, 68, 92	3 (0%)
1	B	499/521 (95%)	0.07	33 (6%)	22	24	25, 41, 71, 96	4 (0%)
1	C	507/521 (97%)	-0.02	24 (4%)	35	40	25, 38, 61, 103	4 (0%)
1	D	504/521 (96%)	-0.07	17 (3%)	49	54	25, 38, 59, 83	1 (0%)
All	All	2010/2084 (96%)	0.01	104 (5%)	31	35	25, 39, 66, 103	12 (0%)

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	183	SER	8.8
1	B	13	ALA	6.3
1	B	63	ASN	5.8
1	B	185	SER	5.0
1	B	62	LYS	5.0
1	A	14	GLU	5.0
1	B	12	VAL	4.8
1	C	113	PRO	4.8
1	A	63	ASN	4.8
1	A	185	SER	4.7
1	D	515	ILE	4.6
1	D	63	ASN	4.5
1	D	185	SER	4.5
1	A	16	THR	4.5
1	D	62	LYS	4.5
1	C	185	SER	4.5
1	D	257	ARG	4.3
1	D	122	ALA	4.3
1	C	122	ALA	4.3
1	C	121	HIS	4.2
1	A	64	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	183	SER	4.0
1	B	61	GLY	3.8
1	C	64	VAL	3.8
1	A	13	ALA	3.7
1	A	11	THR	3.7
1	B	64	VAL	3.6
1	C	111	GLY	3.5
1	B	16	THR	3.5
1	C	114	ASP	3.5
1	A	61	GLY	3.5
1	A	15	GLY	3.4
1	D	110	ASP	3.3
1	C	112	LEU	3.3
1	C	184	GLU	3.3
1	B	11	THR	3.3
1	B	65	LYS	3.2
1	A	514	PRO	3.2
1	B	68	PRO	3.2
1	D	258	THR	3.1
1	A	17	ARG	3.1
1	B	146	PRO	3.1
1	B	15	GLY	3.1
1	B	74	VAL	3.0
1	A	106	GLN	3.0
1	B	514	PRO	3.0
1	B	110	ASP	3.0
1	C	304	THR	3.0
1	B	14	GLU	3.0
1	C	257	ARG	2.9
1	B	123	ASP	2.8
1	C	258	THR	2.8
1	D	11	THR	2.8
1	A	75	VAL	2.8
1	B	109	LEU	2.7
1	C	3	LEU	2.7
1	B	106	GLN	2.7
1	B	75	VAL	2.7
1	B	104	THR	2.7
1	A	12	VAL	2.7
1	B	468	ASN	2.7
1	C	123	ASP	2.6
1	A	515	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	88	PHE	2.6
1	A	62	LYS	2.5
1	B	32	ARG	2.5
1	A	466	TYR	2.5
1	D	123	ASP	2.4
1	B	154	ILE	2.4
1	B	258	THR	2.4
1	A	186	SER	2.4
1	B	513	PRO	2.4
1	B	471	GLU	2.4
1	D	183	SER	2.4
1	D	155	GLY	2.4
1	A	429	LEU	2.3
1	C	11	THR	2.3
1	D	154	ILE	2.3
1	C	39	ARG	2.3
1	A	143	ASN	2.3
1	C	358	ASP	2.2
1	C	15	GLY	2.2
1	B	73	ALA	2.2
1	D	15	GLY	2.2
1	C	109	LEU	2.2
1	A	88	PHE	2.1
1	B	3	LEU	2.1
1	A	146	PRO	2.1
1	B	155	GLY	2.1
1	C	514	PRO	2.1
1	A	38	GLY	2.1
1	B	98	VAL	2.1
1	A	18	LEU	2.1
1	C	490	ARG	2.1
1	D	76	MET	2.1
1	D	490	ARG	2.1
1	A	333	GLU	2.1
1	C	469	HIS	2.1
1	A	87	LYS	2.1
1	C	99	LEU	2.1
1	D	186	SER	2.1
1	A	60	ARG	2.0
1	A	65	LYS	2.0
1	A	155	GLY	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^{th} 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
5	EDO	D	908	4/4	0.90	0.26	10.28	49,50,50,52	0
5	EDO	A	906	4/4	0.72	0.24	6.51	59,59,60,60	0
5	EDO	B	905	4/4	0.82	0.24	5.00	64,64,64,64	0
2	DQ1	C	602	31/31	0.91	0.26	2.59	51,65,81,82	2
2	DQ1	B	602	31/31	0.84	0.29	1.76	76,89,98,98	2
5	EDO	A	902	4/4	0.95	0.19	0.98	39,39,39,40	0
5	EDO	D	903	4/4	0.94	0.20	0.87	40,40,41,42	0
2	DQ1	A	602	31/31	0.91	0.20	0.53	45,51,58,59	2
3	NAP	D	702	48/48	0.93	0.18	0.29	38,42,44,45	0
5	EDO	C	909	4/4	0.96	0.16	0.24	41,41,41,43	0
3	NAP	C	702	48/48	0.91	0.17	0.02	51,59,65,66	0
2	DQ1	D	602	31/31	0.92	0.16	-0.01	35,44,57,57	2
3	NAP	B	702	48/48	0.92	0.16	-0.23	57,66,76,77	0
5	EDO	B	912	4/4	0.95	0.14	-0.48	42,42,43,45	0
4	SO4	B	601	5/5	0.96	0.12	-0.48	69,69,70,71	0
3	NAP	A	702	48/48	0.93	0.16	-0.53	34,41,46,46	0
4	SO4	D	522	5/5	0.96	0.11	-0.77	65,66,66,66	0
4	SO4	C	801	5/5	0.98	0.10	-1.34	66,67,68,69	0
4	SO4	B	701	5/5	0.91	0.57	-	114,115,115,115	0
5	EDO	C	913	4/4	0.92	0.17	-	67,67,67,67	0
4	SO4	A	701	5/5	0.88	0.43	-	100,100,100,100	0
4	SO4	D	601	5/5	0.97	0.12	-	56,56,57,57	0
4	SO4	C	701	5/5	0.81	0.59	-	112,112,112,113	0
5	EDO	D	910	4/4	0.83	0.32	-	58,59,59,59	0
4	SO4	D	701	5/5	0.87	0.45	-	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	EDO	B	904	4/4	0.95	0.14	-	63,63,63,64	0
5	EDO	D	911	4/4	0.93	0.15	-	67,67,67,68	0
5	EDO	A	907	4/4	0.91	0.14	-	77,77,77,77	0
5	EDO	A	901	4/4	0.88	0.11	-	50,51,52,52	0

6.5 Other polymers (i)

There are no such residues in this entry.