



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2018 – 05:51 am GMT

PDB ID : 3RDH
Title : X-ray induced covalent inhibition of 14-3-3
Authors : Horton, J.R.; Upadhyay, A.K.; Fu, H.; Cheng, X.
Deposited on : 2011-04-01
Resolution : 2.39 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk31020
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk31020

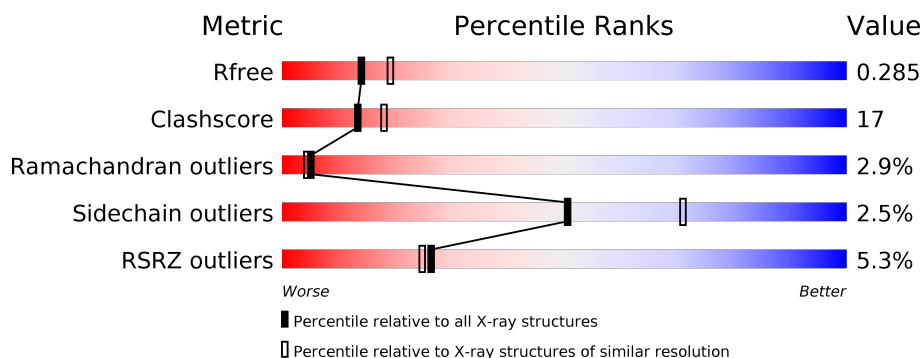
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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}	111664	3481 (2.40-2.40)
Clashscore	122126	3956 (2.40-2.40)
Ramachandran outliers	120053	3897 (2.40-2.40)
Sidechain outliers	120020	3898 (2.40-2.40)
RSRZ outliers	108989	3386 (2.40-2.40)

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	248	<div> <div>3%</div> <div> <div></div> <div>59%</div> <div>33%</div> <div>6%</div> </div> </div>
1	B	248	<div> <div>6%</div> <div> <div></div> <div>60%</div> <div>33%</div> <div>6%</div> </div> </div>
1	C	248	<div> <div>4%</div> <div> <div></div> <div>63%</div> <div>29%</div> <div>6%</div> </div> </div>
1	D	248	<div> <div>6%</div> <div> <div></div> <div>56%</div> <div>35%</div> <div>6%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7471 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.

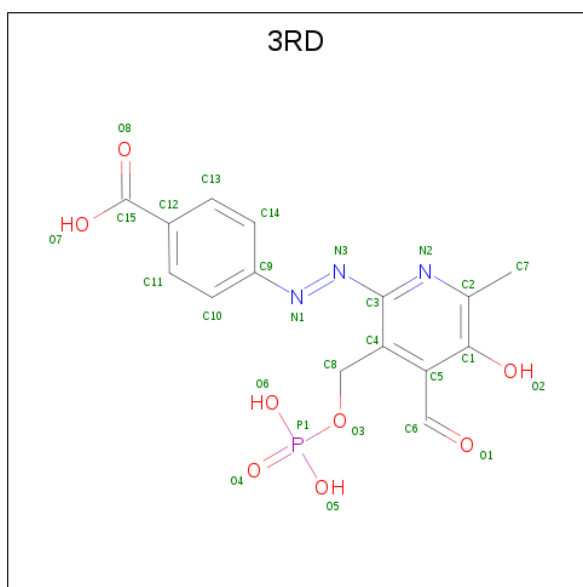
- Molecule 1 is a protein called 14-3-3 protein zeta/delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	S	0	3	0
			1862	1163	316	373	10			
1	B	233	Total	C	N	O	S	0	1	0
			1815	1134	307	364	10			
1	C	233	Total	C	N	O	S	0	0	0
			1820	1136	309	365	10			
1	D	233	Total	C	N	O	S	0	0	0
			1816	1138	304	364	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP P63104
A	-1	SER	-	EXPRESSION TAG	UNP P63104
A	0	HIS	-	EXPRESSION TAG	UNP P63104
B	-2	GLY	-	EXPRESSION TAG	UNP P63104
B	-1	SER	-	EXPRESSION TAG	UNP P63104
B	0	HIS	-	EXPRESSION TAG	UNP P63104
C	-2	GLY	-	EXPRESSION TAG	UNP P63104
C	-1	SER	-	EXPRESSION TAG	UNP P63104
C	0	HIS	-	EXPRESSION TAG	UNP P63104
D	-2	GLY	-	EXPRESSION TAG	UNP P63104
D	-1	SER	-	EXPRESSION TAG	UNP P63104
D	0	HIS	-	EXPRESSION TAG	UNP P63104

- Molecule 2 is 4-[(E)-{4-formyl-5-hydroxy-6-methyl-3-[(phosphonoxy)methyl]pyridin-2-yl}diazanyl]benzoic acid (three-letter code: 3RD) (formula: C₁₅H₁₄N₃O₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			17	8	2	6	1		
2	B	1	Total	C	N	O	P	0	0
			17	8	2	6	1		
2	C	1	Total	C	N	O	P	0	0
			17	8	2	6	1		
2	D	1	Total	C	N	O	P	0	0
			17	8	2	6	1		

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ni	0	0
			1	1		
3	A	1	Total	Ni	0	0
			1	1		
3	D	1	Total	Ni	0	0
			1	1		
3	C	1	Total	Ni	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	21	Total	O	0	0
			21	21		

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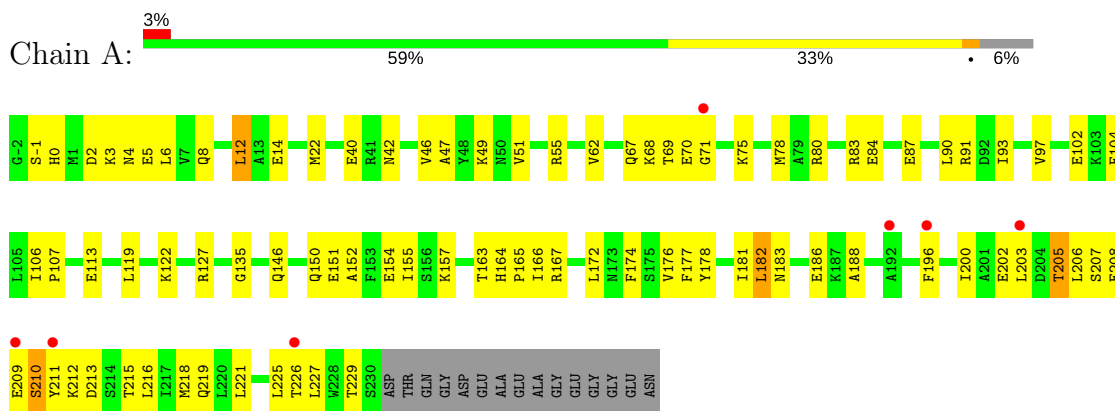
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	24	Total 24	O 24	0	0
4	C	21	Total 21	O 21	0	0
4	D	20	Total 20	O 20	0	0

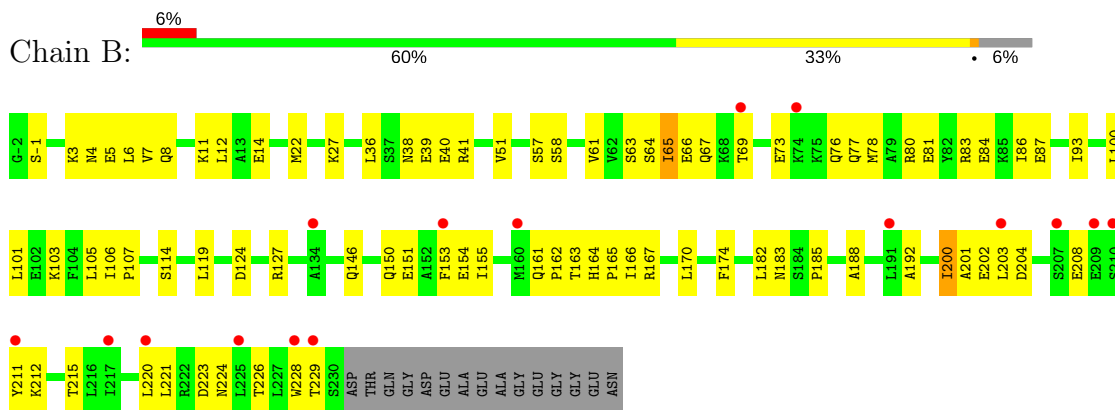
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

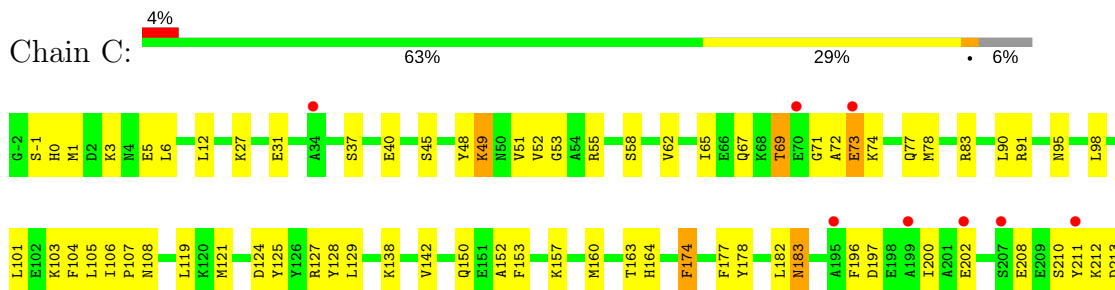
- Molecule 1: 14-3-3 protein zeta/delta



- Molecule 1: 14-3-3 protein zeta/delta

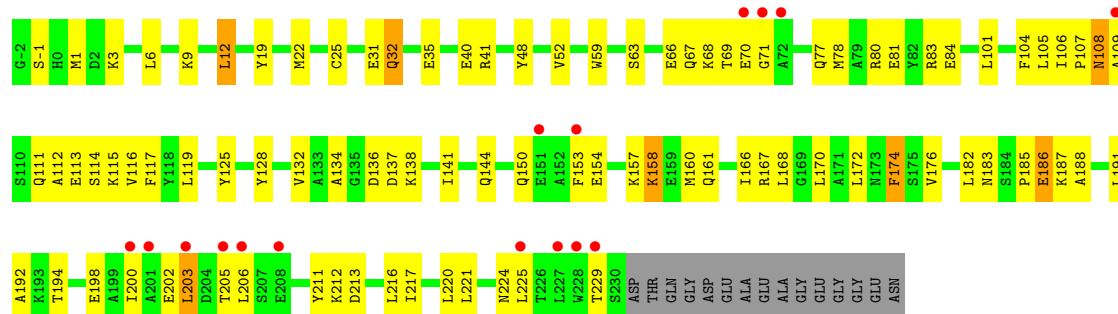


- Molecule 1: 14-3-3 protein zeta/delta





- Molecule 1: 14-3-3 protein zeta/delta



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	94.75Å 94.75Å 237.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	33.77 – 2.39 33.77 – 2.38	Depositor EDS
% Data completeness (in resolution range)	93.8 (33.77-2.39) 93.6 (33.77-2.38)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.39Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.235 , 0.286 0.235 , 0.285	Depositor DCC
R_{free} test set	2369 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	44.0	Xtriage
Anisotropy	0.451	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 34.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.217 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7471	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.48% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: NI, 3RD

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	0.38	0/1888	0.56	0/2543
1	B	0.38	0/1841	0.55	0/2483
1	C	0.36	0/1845	0.54	0/2486
1	D	0.37	0/1842	0.55	0/2485
All	All	0.37	0/7416	0.55	0/9997

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 [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	1862	0	1811	75	0
1	B	1815	0	1738	59	0
1	C	1820	0	1763	57	0
1	D	1816	0	1752	75	0
2	A	17	0	9	0	0
2	B	17	0	9	0	0
2	C	17	0	9	0	0
2	D	17	0	9	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	21	0	0	1	0
4	B	24	0	0	0	0
4	C	21	0	0	1	0
4	D	20	0	0	0	0
All	All	7471	0	7100	251	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 17.

All (251) 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:D:113:GLU:HA	1:D:160:MET:HE3	1.55	0.88
1:C:3:LYS:HA	1:C:6:LEU:HD12	1.63	0.80
1:A:200:ILE:HD13	1:A:203:LEU:HD21	1.62	0.80
1:D:108:ASN:HD22	1:D:108:ASN:N	1.81	0.78
1:B:5:GLU:HG3	1:C:78:MET:HE3	1.66	0.77
1:B:69:THR:O	1:B:76:GLN:HB2	1.87	0.75
1:C:196:PHE:O	1:C:200:ILE:HG13	1.87	0.74
1:D:168:LEU:HB3	1:D:217:ILE:HG21	1.69	0.74
1:C:196:PHE:CE1	1:C:200:ILE:HD11	2.24	0.72
1:A:49:LYS:HD3	1:A:49:LYS:C	2.11	0.71
1:A:226:THR:HA	1:A:229:THR:HG22	1.72	0.70
1:D:202:GLU:O	1:D:205:THR:HG22	1.92	0.70
1:A:127:ARG:HD2	4:A:262:HOH:O	1.91	0.70
1:B:51:VAL:HG12	1:B:93:ILE:HD13	1.73	0.69
1:A:83:ARG:O	1:A:87:GLU:HG3	1.93	0.69
1:A:146:GLN:OE1	1:A:182:LEU:HD11	1.94	0.68
1:C:58:SER:O	1:C:62:VAL:HG23	1.95	0.66
1:D:69:THR:O	1:D:71:GLY:N	2.29	0.65
1:C:138:LYS:HE3	1:C:142:VAL:HG21	1.77	0.65
1:A:212:LYS:O	1:A:216:LEU:HB2	1.96	0.65
1:D:67:GLN:C	1:D:69:THR:H	1.99	0.65
1:D:200:ILE:O	1:D:203:LEU:HB2	1.96	0.65
1:D:192:ALA:HB3	1:D:225:LEU:HD13	1.80	0.64
1:D:80:ARG:O	1:D:84:GLU:HG3	1.98	0.63
1:B:146:GLN:OE1	1:B:182:LEU:HD11	2.00	0.61
1:C:210:SER:HA	1:C:213:ASP:HB2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:VAL:HG22	1:D:12:LEU:HD21	1.82	0.60
1:A:202:GLU:HB3	1:A:205:THR:CG2	2.32	0.60
1:A:172:LEU:O	1:A:176:VAL:HG23	2.03	0.59
1:C:197:ASP:HA	1:C:200:ILE:HD12	1.84	0.58
1:A:55:ARG:HB3	1:A:90:LEU:HG	1.86	0.58
1:C:37:SER:OG	1:C:40:GLU:HG3	2.04	0.58
1:D:67:GLN:O	1:D:69:THR:N	2.37	0.58
1:C:208:GLU:C	1:C:210:SER:H	2.06	0.57
1:D:216:LEU:O	1:D:220:LEU:HG	2.05	0.57
1:C:49:LYS:HE3	1:C:49:LYS:HA	1.87	0.57
1:A:106:ILE:HB	1:A:107:PRO:HD3	1.85	0.57
1:A:51:VAL:HG12	1:A:93:ILE:HD13	1.86	0.57
1:D:172:LEU:O	1:D:176:VAL:HG23	2.05	0.57
1:A:150:GLN:O	1:A:154:GLU:HG2	2.05	0.57
1:A:178:TYR:CD1	1:A:182:LEU:HD12	2.40	0.57
1:B:78:MET:HE1	1:C:5:GLU:HB3	1.87	0.57
1:B:221:LEU:O	1:B:221:LEU:HD23	2.05	0.57
1:C:101:LEU:HD23	1:C:105:LEU:HD12	1.87	0.57
1:D:66:GLU:CD	1:D:83:ARG:HE	2.08	0.57
1:B:220[A]:LEU:HA	1:B:223:ASP:OD2	2.06	0.56
1:D:112:ALA:O	1:D:116:VAL:HG23	2.04	0.56
1:D:108:ASN:ND2	1:D:108:ASN:N	2.54	0.55
1:D:153:PHE:HA	1:D:170:LEU:HD21	1.89	0.55
1:D:48:TYR:O	1:D:52:VAL:HG12	2.06	0.55
1:A:157:LYS:HD2	1:A:167:ARG:NH2	2.21	0.55
1:A:202:GLU:HB3	1:A:205:THR:HB	1.88	0.55
1:D:77:GLN:O	1:D:81:GLU:HG3	2.05	0.55
1:B:64:SER:O	1:B:65:ILE:C	2.45	0.55
1:C:174:PHE:O	1:C:177:PHE:HB3	2.08	0.54
1:B:38:ASN:OD1	1:B:39:GLU:N	2.34	0.54
1:C:1:MET:HE2	4:C:259:HOH:O	2.07	0.54
1:C:65:ILE:HG22	1:C:65:ILE:O	2.08	0.54
1:B:73:GLU:O	1:B:77:GLN:HB2	2.07	0.54
1:B:77:GLN:O	1:B:81:GLU:HG3	2.07	0.54
1:A:207:SER:O	1:A:211:TYR:N	2.41	0.53
1:B:106:ILE:HB	1:B:107:PRO:HD3	1.91	0.53
1:D:211:TYR:CE2	1:D:212:LYS:HG3	2.43	0.53
1:A:3:LYS:HA	1:A:6:LEU:HD12	1.90	0.53
1:B:162:PRO:HG3	1:B:167:ARG:NH2	2.22	0.53
1:D:41:ARG:NH1	1:D:114:SER:HB3	2.24	0.53
1:D:221:LEU:O	1:D:225:LEU:HB2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:LEU:O	1:D:206:LEU:HG	2.09	0.53
1:A:2:ASP:OD1	1:A:5:GLU:HB2	2.09	0.53
1:C:196:PHE:CD1	1:C:200:ILE:HD11	2.44	0.53
1:D:150:GLN:O	1:D:154:GLU:HG2	2.09	0.53
1:D:67:GLN:C	1:D:69:THR:N	2.63	0.53
1:A:215:THR:HA	1:A:218:MET:HB2	1.90	0.52
1:A:67:GLN:C	1:A:69:THR:H	2.13	0.52
1:D:35:GLU:OE2	1:D:109:ALA:HA	2.08	0.52
1:D:9:LYS:HG3	1:D:25:CYS:SG	2.49	0.52
1:C:163:THR:CG2	1:C:202:GLU:HB2	2.40	0.52
1:A:202:GLU:O	1:A:205:THR:HG22	2.09	0.52
1:B:224:ASN:HB3	1:B:228:TRP:CZ2	2.45	0.52
1:A:208:GLU:HA	1:A:211:TYR:HD2	1.75	0.52
1:A:200:ILE:HA	1:A:203:LEU:HG	1.91	0.52
1:B:220[B]:LEU:HA	1:B:223:ASP:OD2	2.10	0.52
1:C:74:LYS:O	1:C:77:GLN:HB3	2.10	0.52
1:C:104:PHE:O	1:C:108:ASN:HB2	2.10	0.52
1:D:106:ILE:HB	1:D:107:PRO:HD3	1.92	0.52
1:B:36:LEU:HB3	1:B:40:GLU:HB2	1.92	0.51
1:C:212:LYS:O	1:C:216:LEU:HD13	2.10	0.51
1:D:185:PRO:HA	1:D:188:ALA:HB3	1.92	0.51
1:D:211:TYR:CZ	1:D:212:LYS:HG3	2.45	0.51
1:B:4:ASN:O	1:B:8:GLN:HG2	2.11	0.51
1:A:208:GLU:OE1	1:A:208:GLU:N	2.41	0.51
1:A:4:ASN:O	1:A:8[A]:GLN:HG3	2.10	0.51
1:D:59:TRP:CE2	1:D:132:VAL:HG12	2.46	0.51
1:B:78:MET:HE3	1:C:5:GLU:HG2	1.92	0.51
1:D:107:PRO:C	1:D:108:ASN:HD22	2.15	0.51
1:D:185:PRO:HG2	1:D:186:GLU:OE2	2.11	0.50
1:A:210:SER:HA	1:A:213:ASP:OD2	2.11	0.50
1:B:185:PRO:HA	1:B:188:ALA:HB3	1.92	0.50
1:B:41:ARG:HH11	1:B:114:SER:HB3	1.77	0.50
1:B:63:SER:O	1:B:67:GLN:HG2	2.12	0.50
1:D:157:LYS:O	1:D:157:LYS:HG2	2.12	0.50
1:D:158:LYS:O	1:D:158:LYS:HG2	2.11	0.50
1:A:80:ARG:HG3	1:A:83:ARG:HH21	1.76	0.50
1:D:160:MET:O	1:D:167:ARG:NH1	2.44	0.49
1:D:168:LEU:HB3	1:D:217:ILE:CG2	2.39	0.49
1:A:113:GLU:OE1	1:A:164:HIS:HE1	1.94	0.49
1:B:64:SER:O	1:B:67:GLN:N	2.45	0.49
1:A:200:ILE:O	1:A:203:LEU:HG	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ARG:O	1:A:84:GLU:HG3	2.11	0.49
1:B:77:GLN:HE21	1:B:80:ARG:NH2	2.11	0.49
1:C:119:LEU:HB3	1:C:152:ALA:HB2	1.93	0.49
1:C:0:HIS:CD2	1:C:1:MET:HG3	2.48	0.49
1:A:14:GLU:HB2	1:A:22:MET:SD	2.53	0.49
1:D:3:LYS:HB2	1:D:32:GLN:HG2	1.95	0.49
1:A:151:GLU:O	1:A:155:ILE:HG13	2.13	0.49
1:B:57:SER:O	1:B:61:VAL:HG23	2.13	0.48
1:B:5:GLU:HG3	1:C:78:MET:CE	2.41	0.48
1:C:157:LYS:HG3	1:C:157:LYS:O	2.12	0.48
1:C:51:VAL:HG13	1:C:55:ARG:NH1	2.28	0.48
1:B:78:MET:CE	1:C:5:GLU:HB3	2.43	0.48
1:D:161:GLN:O	1:D:167:ARG:HD3	2.13	0.48
1:B:202:GLU:C	1:B:204:ASP:H	2.16	0.48
1:B:73:GLU:OE1	1:B:73:GLU:HA	2.13	0.48
1:B:202:GLU:C	1:B:204:ASP:N	2.67	0.48
1:A:164:HIS:CD2	1:A:165:PRO:HD2	2.48	0.48
1:A:215:THR:O	1:A:219:GLN:HG3	2.14	0.48
1:B:153:PHE:HA	1:B:170:LEU:HD21	1.96	0.48
1:A:42:ASN:O	1:A:46:VAL:HG23	2.14	0.47
1:D:3:LYS:NZ	1:D:40:GLU:OE2	2.39	0.47
1:D:80:ARG:HG3	1:D:83:ARG:NH2	2.28	0.47
1:A:181:ILE:C	1:A:183[A]:ASN:H	2.17	0.47
1:D:172:LEU:HD11	1:D:224:ASN:ND2	2.29	0.47
1:B:200:ILE:C	1:B:202:GLU:H	2.18	0.47
1:C:210:SER:O	1:C:211:TYR:C	2.53	0.47
1:B:14:GLU:HB2	1:B:22:MET:SD	2.54	0.47
1:B:3:LYS:HA	1:B:6:LEU:HD12	1.96	0.47
1:B:101:LEU:HD23	1:B:105:LEU:HD12	1.96	0.47
1:A:49:LYS:O	1:A:49:LYS:HD3	2.13	0.47
1:C:55:ARG:N	1:C:55:ARG:HD2	2.30	0.47
1:A:163:THR:HB	1:A:206:LEU:HD23	1.97	0.47
1:A:221:LEU:O	1:A:225:LEU:HB2	2.15	0.47
1:B:164:HIS:HD2	1:B:166:ILE:H	1.63	0.47
1:A:104:PHE:CZ	1:C:103:LYS:HG3	2.50	0.47
1:B:36:LEU:HD22	1:B:40:GLU:HB3	1.96	0.46
1:B:80:ARG:HG2	1:B:84:GLU:OE2	2.15	0.46
1:B:83:ARG:NH1	1:B:87:GLU:OE2	2.47	0.46
1:C:98:LEU:HA	1:C:101:LEU:HD12	1.95	0.46
1:A:178:TYR:HD1	1:A:182:LEU:HD12	1.80	0.46
1:C:210:SER:HB3	1:C:214:SER:OG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:GLN:HE21	1:A:154:GLU:CD	2.19	0.46
1:C:227:LEU:C	1:C:229:THR:H	2.18	0.46
1:A:93:ILE:O	1:A:97:VAL:HG23	2.15	0.46
1:D:200:ILE:HG23	1:D:203:LEU:HD12	1.97	0.46
1:B:203:LEU:HD21	1:B:215:THR:CG2	2.46	0.46
1:C:160:MET:HE3	1:C:164:HIS:CE1	2.50	0.46
1:D:125:TYR:HA	1:D:128:TYR:CD2	2.51	0.46
1:C:48:TYR:O	1:C:52:VAL:HG12	2.15	0.46
1:A:182:LEU:O	1:A:183[B]:ASN:C	2.54	0.46
1:A:67:GLN:O	1:A:69:THR:N	2.49	0.46
1:A:3:LYS:NZ	1:A:40:GLU:OE2	2.47	0.45
1:B:66:GLU:OE2	1:B:80:ARG:HG3	2.16	0.45
1:A:227:LEU:O	1:A:227:LEU:HD12	2.16	0.45
1:D:170:LEU:O	1:D:174:PHE:HB2	2.16	0.45
1:C:208:GLU:C	1:C:210:SER:N	2.69	0.45
1:D:115:LYS:HB2	1:D:115:LYS:HE3	1.77	0.45
1:A:62:VAL:HG22	1:D:12:LEU:CD2	2.46	0.45
1:C:3:LYS:O	1:C:6:LEU:HB2	2.17	0.45
1:B:174:PHE:CD1	1:B:174:PHE:O	2.70	0.45
1:C:3:LYS:NZ	1:C:40:GLU:OE2	2.49	0.45
1:D:41:ARG:HH11	1:D:114:SER:HB3	1.82	0.45
1:C:67:GLN:C	1:C:69:THR:H	2.20	0.45
1:A:78:MET:SD	1:D:12:LEU:HD12	2.57	0.45
1:A:102:GLU:OE1	1:A:122:LYS:HE3	2.17	0.45
1:A:202:GLU:HB3	1:A:205:THR:CB	2.47	0.45
1:D:1:MET:HE3	1:D:6:LEU:HD11	1.99	0.45
1:C:71:GLY:O	1:C:73:GLU:N	2.50	0.44
1:B:103:LYS:HE3	1:D:31:GLU:O	2.17	0.44
1:A:177:PHE:O	1:A:181:ILE:HB	2.17	0.44
1:B:153:PHE:CA	1:B:170:LEU:HD21	2.47	0.44
1:A:119:LEU:HB3	1:A:152:ALA:HB2	1.98	0.44
1:A:119:LEU:CB	1:A:152:ALA:HB2	2.47	0.44
1:B:27:LYS:HG3	1:B:100:LEU:HD11	1.98	0.44
1:A:157:LYS:HG3	1:A:157:LYS:O	2.18	0.44
1:A:87:GLU:O	1:A:91:ARG:HG3	2.17	0.44
1:D:101:LEU:HD23	1:D:105:LEU:HD12	2.00	0.44
1:A:8[A]:GLN:HB2	1:D:78:MET:HE2	2.00	0.44
1:A:181:ILE:C	1:A:183[B]:ASN:H	2.19	0.44
1:B:164:HIS:CD2	1:B:165:PRO:HD2	2.53	0.44
1:C:106:ILE:HB	1:C:107:PRO:HD3	2.00	0.43
1:B:66:GLU:CD	1:B:83:ARG:HE	2.20	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:GLU:OE2	1:D:80:ARG:HA	2.18	0.43
1:A:182:LEU:O	1:A:183[A]:ASN:C	2.55	0.43
1:A:196:PHE:O	1:A:200:ILE:HG12	2.18	0.43
1:D:117:PHE:HB2	1:D:166:ILE:HD13	1.99	0.43
1:C:208:GLU:HA	1:C:211:TYR:CB	2.48	0.43
1:D:194:THR:HG22	1:D:198:GLU:OE2	2.18	0.43
1:D:113:GLU:HG3	1:D:160:MET:CE	2.48	0.43
1:A:202:GLU:O	1:A:205:THR:N	2.43	0.43
1:B:119:LEU:HD12	1:B:155:ILE:HD12	2.01	0.43
1:D:182:LEU:HA	1:D:182:LEU:HD23	1.87	0.43
1:B:7:VAL:HG12	1:B:11:LYS:HE3	2.01	0.43
1:C:150:GLN:O	1:C:153:PHE:HB3	2.19	0.43
1:A:163:THR:HG21	1:A:205:THR:HG22	2.00	0.43
1:B:150:GLN:O	1:B:154:GLU:HG2	2.18	0.43
1:C:125:TYR:HA	1:C:128:TYR:CD2	2.54	0.42
1:C:178:TYR:CD1	1:C:182:LEU:HD12	2.54	0.42
1:A:200:ILE:HA	1:A:203:LEU:CD2	2.49	0.42
1:C:119:LEU:CB	1:C:152:ALA:HB2	2.49	0.42
1:B:211:TYR:CG	1:B:212:LYS:N	2.86	0.42
1:C:91:ARG:HA	1:C:129:LEU:HD21	2.01	0.42
1:B:226:THR:HA	1:B:229:THR:OG1	2.20	0.42
1:D:101:LEU:HA	1:D:105:LEU:HB2	2.01	0.42
1:D:229:THR:O	1:D:229:THR:HG22	2.20	0.42
1:A:0:HIS:HD2	1:C:95:ASN:OD1	2.03	0.42
1:A:207:SER:C	1:A:209:GLU:N	2.73	0.42
1:D:134:ALA:O	1:D:138:LYS:HB2	2.20	0.42
1:D:141:ILE:O	1:D:144:GLN:HB2	2.19	0.42
1:C:27:LYS:O	1:C:31:GLU:HG3	2.19	0.42
1:C:45:SER:O	1:C:49:LYS:HB2	2.20	0.42
1:C:52:VAL:HG13	1:C:53:GLY:N	2.35	0.42
1:D:41:ARG:HH11	1:D:114:SER:CB	2.33	0.42
1:D:203:LEU:O	1:D:203:LEU:HD23	2.19	0.42
1:A:67:GLN:C	1:A:69:THR:N	2.73	0.41
1:B:8:GLN:HB2	1:C:78:MET:HE1	2.02	0.41
1:B:8:GLN:HB2	1:C:78:MET:CE	2.51	0.41
1:D:106:ILE:HD13	1:D:119:LEU:HD23	2.02	0.41
1:D:168:LEU:CB	1:D:217:ILE:HG21	2.44	0.41
1:B:151:GLU:O	1:B:155:ILE:HG13	2.19	0.41
1:D:153:PHE:CA	1:D:170:LEU:HD21	2.51	0.41
1:D:19:TYR:HA	1:D:22:MET:HB3	2.02	0.41
1:A:164:HIS:HD2	1:A:166:ILE:H	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:ASP:O	1:C:127:ARG:HB3	2.20	0.41
1:D:1:MET:HG3	1:D:32:GLN:HE22	1.86	0.41
1:A:22:MET:HG2	1:A:47:ALA:HB2	2.02	0.41
1:B:124:ASP:O	1:B:127:ARG:HB3	2.21	0.41
1:D:32:GLN:OE1	1:D:32:GLN:HA	2.20	0.41
1:A:163:THR:HB	1:A:206:LEU:CD2	2.51	0.41
1:B:224:ASN:HB3	1:B:228:TRP:CE2	2.56	0.41
1:B:161:GLN:NE2	1:B:163:THR:OG1	2.54	0.40
1:C:83:ARG:HG2	1:C:83:ARG:HH11	1.87	0.40
1:A:75:LYS:O	1:A:78:MET:HB3	2.21	0.40
1:B:58:SER:HB3	1:B:86:ILE:HD13	2.03	0.40
1:D:31:GLU:HA	1:D:104:PHE:CE2	2.56	0.40
1:D:211:TYR:OH	1:D:212:LYS:HE2	2.21	0.40
1:A:70:GLU:O	1:A:71:GLY:C	2.60	0.40
1:C:157:LYS:CG	1:C:157:LYS:O	2.69	0.40
1:A:12:LEU:HD12	1:D:78:MET:SD	2.62	0.40
1:A:226:THR:CA	1:A:229:THR:HG22	2.45	0.40
1:B:203:LEU:HD12	1:B:203:LEU:HA	1.93	0.40
1:D:186:GLU:HB2	1:D:187:LYS:H	1.79	0.40
1:D:63:SER:O	1:D:66:GLU:HB3	2.22	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	234/248 (94%)	203 (87%)	24 (10%)	7 (3%)	5	4
1	B	232/248 (94%)	207 (89%)	18 (8%)	7 (3%)	5	4
1	C	231/248 (93%)	209 (90%)	17 (7%)	5 (2%)	7	8
1	D	231/248 (93%)	208 (90%)	15 (6%)	8 (4%)	4	3
All	All	928/992 (94%)	827 (89%)	74 (8%)	27 (3%)	5	4

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	-1	SER
1	C	69	THR
1	C	72	ALA
1	A	-1	SER
1	A	68	LYS
1	A	135	GLY
1	A	188	ALA
1	B	-1	SER
1	B	183	ASN
1	B	201	ALA
1	D	-1	SER
1	D	68	LYS
1	D	70	GLU
1	D	158	LYS
1	D	186	GLU
1	A	186	GLU
1	A	210	SER
1	B	208	GLU
1	C	73	GLU
1	C	183	ASN
1	B	65	ILE
1	D	136	ASP
1	A	182	LEU
1	B	192	ALA
1	D	203	LEU
1	D	183	ASN
1	B	200	ILE

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	198/211 (94%)	195 (98%)	3 (2%)	67	83
1	B	188/211 (89%)	187 (100%)	1 (0%)	90	96
1	C	191/211 (90%)	184 (96%)	7 (4%)	37	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	190/211 (90%)	182 (96%)	8 (4%)	32 51
All	All	767/844 (91%)	748 (98%)	19 (2%)	50 71

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

Mol	Chain	Res	Type
1	A	12	LEU
1	A	174	PHE
1	A	205	THR
1	B	12	LEU
1	C	12	LEU
1	C	49	LYS
1	C	90	LEU
1	C	121	MET
1	C	174	PHE
1	C	183	ASN
1	C	222	ARG
1	D	12	LEU
1	D	32	GLN
1	D	108	ASN
1	D	111	GLN
1	D	137	ASP
1	D	174	PHE
1	D	191	LEU
1	D	213	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	108	ASN
1	A	150	GLN
1	A	164	HIS
1	B	32	GLN
1	B	77	GLN
1	B	108	ASN
1	B	161	GLN
1	B	164	HIS
1	B	224	ASN
1	C	32	GLN
1	C	108	ASN

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Mol	Chain	Res	Type
1	C	111	GLN
1	C	146	GLN
1	C	150	GLN
1	C	164	HIS
1	D	77	GLN
1	D	108	ASN
1	D	224	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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	3RD	A	246	1	16,17,28	2.20	6 (37%)	19,25,40	2.36	6 (31%)
2	3RD	B	246	1	16,17,28	2.13	5 (31%)	19,25,40	2.27	5 (26%)
2	3RD	C	246	1	16,17,28	2.07	6 (37%)	19,25,40	2.15	5 (26%)
2	3RD	D	246	1	16,17,28	2.14	6 (37%)	19,25,40	2.26	5 (26%)

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	3RD	A	246	1	-	0/8/8/17	0/1/1/2
2	3RD	B	246	1	-	0/8/8/17	0/1/1/2
2	3RD	C	246	1	-	0/8/8/17	0/1/1/2
2	3RD	D	246	1	-	0/8/8/17	0/1/1/2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	246	3RD	C7-C2	2.04	1.54	1.50
2	A	246	3RD	C7-C2	2.11	1.54	1.50
2	C	246	3RD	C5-C1	2.26	1.44	1.40
2	D	246	3RD	C7-C2	2.27	1.54	1.50
2	C	246	3RD	C8-C4	2.47	1.55	1.51
2	D	246	3RD	C5-C1	2.52	1.44	1.40
2	B	246	3RD	C8-C4	2.56	1.55	1.51
2	A	246	3RD	C8-C4	2.63	1.56	1.51
2	A	246	3RD	C5-C1	2.76	1.45	1.40
2	B	246	3RD	C5-C1	2.84	1.45	1.40
2	D	246	3RD	C8-C4	2.89	1.56	1.51
2	B	246	3RD	C5-C4	2.97	1.45	1.41
2	C	246	3RD	C5-C4	3.22	1.45	1.41
2	D	246	3RD	C5-C4	3.36	1.46	1.41
2	C	246	3RD	C1-C2	3.38	1.43	1.40
2	A	246	3RD	C1-C2	3.42	1.43	1.40
2	A	246	3RD	C5-C4	3.54	1.46	1.41
2	D	246	3RD	C1-C2	3.72	1.43	1.40
2	B	246	3RD	C1-C2	3.85	1.43	1.40
2	D	246	3RD	C5-C6	4.23	1.56	1.46
2	B	246	3RD	C5-C6	4.26	1.56	1.46
2	C	246	3RD	C5-C6	4.42	1.56	1.46
2	A	246	3RD	C5-C6	4.47	1.57	1.46

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	246	3RD	O3-C8-C4	-7.25	95.76	109.36
2	B	246	3RD	O3-C8-C4	-6.60	96.99	109.36
2	D	246	3RD	O3-C8-C4	-6.20	97.75	109.36
2	C	246	3RD	O3-C8-C4	-6.01	98.10	109.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	246	3RD	N3-C3-N2	-4.73	110.23	117.01
2	A	246	3RD	N3-C3-N2	-4.32	110.81	117.01
2	B	246	3RD	N3-C3-N2	-4.26	110.90	117.01
2	C	246	3RD	N3-C3-N2	-4.08	111.16	117.01
2	C	246	3RD	C5-C1-C2	-3.11	118.24	120.15
2	A	246	3RD	C5-C1-C2	-3.07	118.27	120.15
2	B	246	3RD	C5-C1-C2	-2.99	118.32	120.15
2	D	246	3RD	C5-C1-C2	-2.89	118.38	120.15
2	B	246	3RD	O1-C6-C5	-2.70	118.96	125.09
2	D	246	3RD	O1-C6-C5	-2.64	119.09	125.09
2	C	246	3RD	O1-C6-C5	-2.40	119.63	125.09
2	A	246	3RD	O1-C6-C5	-2.28	119.91	125.09
2	A	246	3RD	O3-P1-O4	2.14	112.48	106.47
2	B	246	3RD	C3-N2-C2	2.46	123.32	119.73
2	A	246	3RD	C3-N2-C2	2.52	123.40	119.73
2	C	246	3RD	C3-N2-C2	2.60	123.52	119.73
2	D	246	3RD	C3-N2-C2	2.66	123.60	119.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	233/248 (93%)	0.48	7 (3%) 50 48	26, 50, 85, 93	0
1	B	233/248 (93%)	0.49	16 (6%) 17 15	27, 56, 100, 115	0
1	C	233/248 (93%)	0.48	10 (4%) 35 33	34, 54, 94, 113	0
1	D	233/248 (93%)	0.56	16 (6%) 17 15	32, 58, 103, 112	0
All	All	932/992 (93%)	0.50	49 (5%) 26 25	26, 55, 96, 115	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	206	LEU	5.8
1	A	71	GLY	4.8
1	A	209	GLU	4.7
1	B	210	SER	4.5
1	C	207	SER	4.3
1	D	205	THR	4.0
1	B	209	GLU	3.8
1	D	225	LEU	3.8
1	D	228	TRP	3.6
1	D	200	ILE	3.6
1	C	70	GLU	3.5
1	D	203	LEU	3.4
1	C	211	TYR	3.4
1	D	72	ALA	3.3
1	A	211	TYR	3.2
1	B	203	LEU	3.1
1	B	229	THR	3.0
1	A	203	LEU	2.9
1	C	73	GLU	2.9
1	B	191	LEU	2.8
1	B	225	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	196	PHE	2.7
1	C	199	ALA	2.6
1	C	195	ALA	2.6
1	D	71	GLY	2.6
1	B	160	MET	2.6
1	D	227	LEU	2.6
1	B	74	LYS	2.6
1	B	134	ALA	2.6
1	C	227	LEU	2.5
1	D	153	PHE	2.5
1	B	220[A]	LEU	2.5
1	C	34	ALA	2.4
1	D	201	ALA	2.4
1	D	229	THR	2.4
1	D	70	GLU	2.3
1	B	207	SER	2.2
1	C	216	LEU	2.2
1	B	228	TRP	2.2
1	C	202	GLU	2.2
1	D	208	GLU	2.2
1	B	153	PHE	2.1
1	B	69	THR	2.1
1	D	109	ALA	2.1
1	A	192	ALA	2.1
1	B	211	TYR	2.0
1	D	151	GLU	2.0
1	B	217	ILE	2.0
1	A	226	THR	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. 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	B-factors(Å ²)	Q<0.9
2	3RD	B	246	17/27	0.89	0.14	62,66,74,74	0
2	3RD	C	246	17/27	0.90	0.15	64,70,74,75	0
2	3RD	D	246	17/27	0.92	0.16	65,71,78,78	0
2	3RD	A	246	17/27	0.94	0.13	58,62,69,70	0
3	NI	D	247	1/1	0.98	0.19	48,48,48,48	0
3	NI	B	247	1/1	0.98	0.19	50,50,50,50	0
3	NI	C	247	1/1	0.99	0.18	42,42,42,42	0
3	NI	A	247	1/1	1.00	0.20	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.