



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 09:00 am GMT

PDB ID : 1JQH
Title : IGF-1 receptor kinase domain
Authors : Pautsch, A.; Zoephel, A.; Ahorn, H.; Spevak, W.; Hauptmann, R.; Nar, H.
Deposited on : 2001-08-07
Resolution : 2.10 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

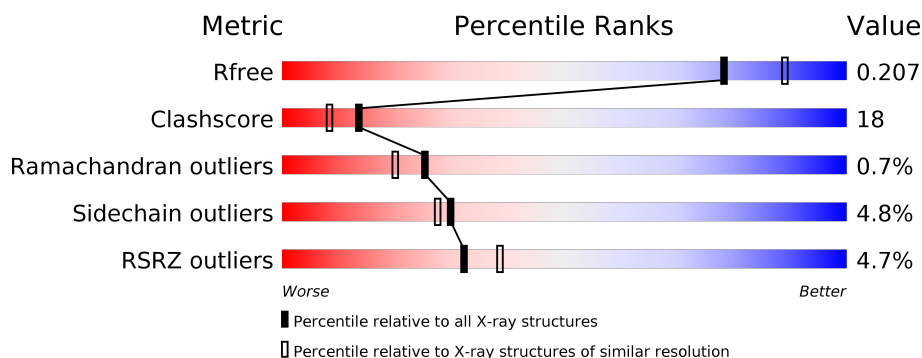
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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	308	<div> <div>5%</div> <div> <div></div> <div>66%</div> <div>27%</div> <div>• 6%</div> </div> </div>
1	B	308	<div> <div>4%</div> <div> <div></div> <div>63%</div> <div>27%</div> <div>• 7%</div> </div> </div>
1	C	308	<div> <div>5%</div> <div> <div></div> <div>63%</div> <div>29%</div> <div>• 6%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	305	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7292 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 IGF-1 receptor kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	0	0	0
			2320	1477	387	434	22			
1	B	287	Total	C	N	O	S	0	0	0
			2291	1458	383	428	22			
1	C	291	Total	C	N	O	S	0	0	0
			2320	1477	387	434	22			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	979	GLY	GLU	ENGINEERED	UNP P08069
A	980	SER	TYR	ENGINEERED	UNP P08069
B	979	GLY	GLU	ENGINEERED	UNP P08069
B	980	SER	TYR	ENGINEERED	UNP P08069
C	979	GLY	GLU	ENGINEERED	UNP P08069
C	980	SER	TYR	ENGINEERED	UNP P08069

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

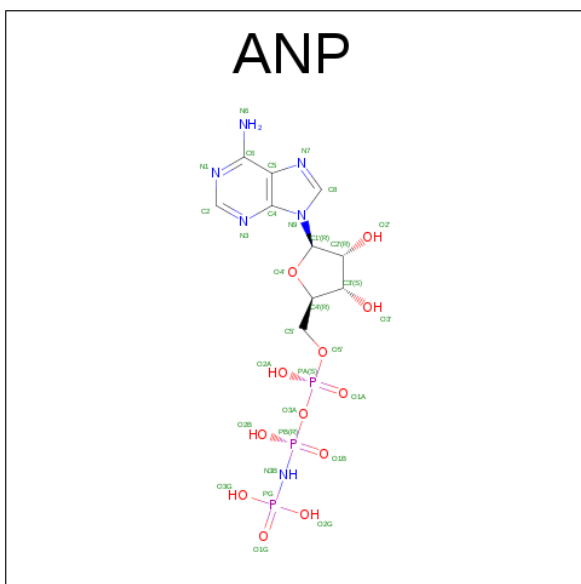
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

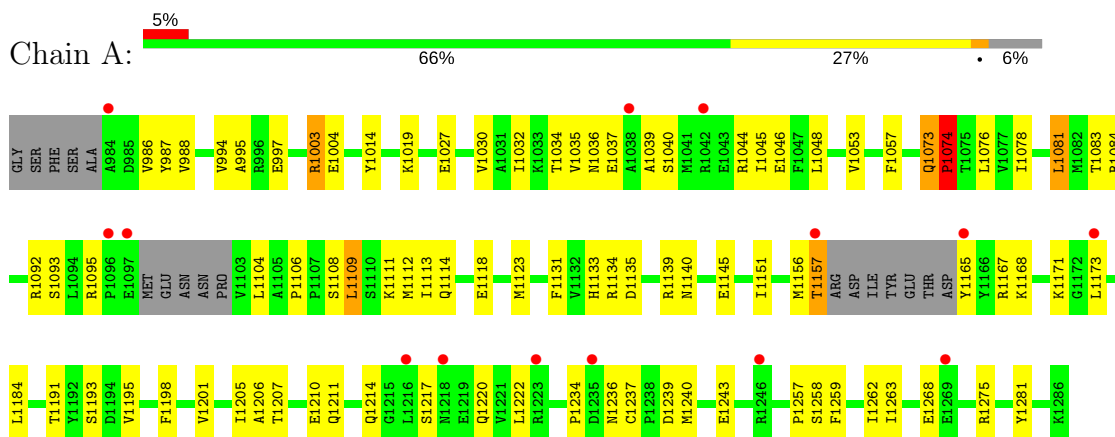
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	84	Total	O	0	0
			84	84		
5	B	91	Total	O	0	0
			91	91		
5	C	77	Total	O	0	0
			77	77		

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 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.

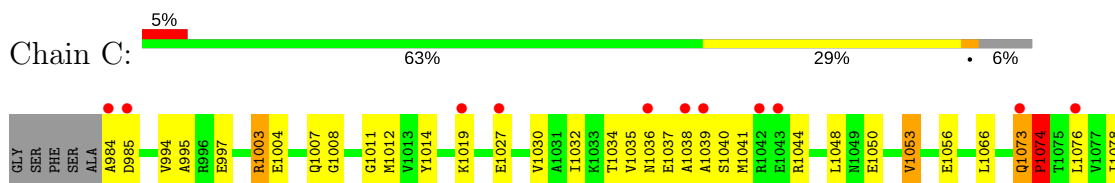
- Molecule 1: IGF-1 receptor kinase

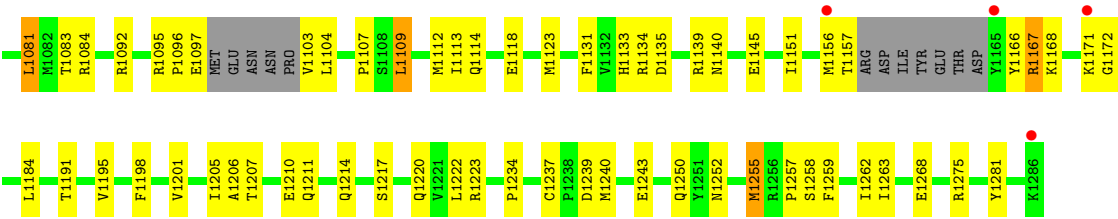


- Molecule 1: IGF-1 receptor kinase



- Molecule 1: IGF-1 receptor kinase





4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	85.96Å 85.96Å 132.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.85 – 2.10 19.84 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.85-2.10) 98.7 (19.84-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.01Å)	Xtriage
Refinement program	CNX 2000	Depositor
R, R_{free}	0.195 , 0.219 0.191 , 0.207	Depositor DCC
R_{free} test set	3054 reflections (5.08%)	DCC
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.380	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.085 for -h,-k,l 0.288 for h,-h-k,-l 0.088 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7292	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ANP, 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	0.41	0/2368	0.78	4/3190 (0.1%)
1	B	0.41	0/2339	0.76	3/3149 (0.1%)
1	C	0.41	0/2368	0.78	3/3190 (0.1%)
All	All	0.41	0/7075	0.77	10/9529 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1073	GLN	C-N-CD	-20.49	75.52	120.60
1	C	1073	GLN	C-N-CD	-20.31	75.92	120.60
1	B	1073	GLN	C-N-CD	-20.04	76.52	120.60
1	A	1073	GLN	C-N-CA	10.14	164.60	122.00
1	C	1073	GLN	C-N-CA	9.81	163.19	122.00
1	B	1073	GLN	C-N-CA	9.52	161.97	122.00
1	B	1074	PRO	CA-N-CD	-8.30	99.88	111.50
1	A	1074	PRO	CA-N-CD	-8.29	99.90	111.50
1	C	1074	PRO	CA-N-CD	-7.16	101.47	111.50
1	A	1106	PRO	C-N-CA	-5.33	99.60	122.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	1223	ARG	Sidechain

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	2320	0	2295	84	0
1	B	2291	0	2265	88	0
1	C	2320	0	2295	93	0
2	A	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	1	0
4	A	31	0	13	0	0
4	B	31	0	13	1	0
4	C	31	0	13	1	0
5	A	84	0	0	6	0
5	B	91	0	0	2	0
5	C	77	0	0	0	0
All	All	7292	0	6894	249	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 18.

All (249) 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:1053:VAL:HG12	1:C:1156:MET:CE	1.78	1.14
1:C:1092:ARG:HH21	1:C:1095:ARG:NE	1.48	1.11
1:C:1053:VAL:HG12	1:C:1156:MET:HE2	1.38	1.04
1:A:1157:THR:HG21	1:C:984:ALA:HA	1.37	1.02
1:B:1003:ARG:HG3	1:B:1003:ARG:HH11	1.28	0.93
1:A:1157:THR:HG21	1:C:984:ALA:CA	2.02	0.90
1:B:1092:ARG:HH21	1:B:1095:ARG:NE	1.69	0.89
1:B:1045:ILE:HD11	1:C:1172:GLY:HA2	1.55	0.89
1:C:1053:VAL:HG12	1:C:1156:MET:HE3	1.53	0.88
1:C:1050:GLU:O	1:C:1053:VAL:HG22	1.75	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1095:ARG:HH22	1:A:1210:GLU:HG2	1.41	0.84
1:A:1104:LEU:N	1:A:1104:LEU:HD22	1.96	0.81
1:A:1003:ARG:HH11	1:A:1003:ARG:HG3	1.42	0.81
1:A:986:VAL:HG23	1:B:1172:GLY:O	1.82	0.80
1:C:1092:ARG:HH21	1:C:1095:ARG:HE	1.28	0.78
1:C:1167:ARG:HH11	1:C:1167:ARG:HB2	1.46	0.77
1:B:1184:LEU:HD22	1:B:1222:LEU:HD22	1.67	0.77
1:C:1184:LEU:HD22	1:C:1222:LEU:HD22	1.67	0.76
1:C:1092:ARG:HH21	1:C:1095:ARG:CZ	1.99	0.76
1:B:1234:PRO:HB2	1:B:1237:CYS:HB2	1.69	0.75
1:C:1003:ARG:HG3	1:C:1003:ARG:HH11	1.51	0.75
1:A:1184:LEU:HD22	1:A:1222:LEU:HD22	1.69	0.75
1:B:1092:ARG:HH21	1:B:1095:ARG:CZ	1.99	0.75
1:A:987:TYR:HB3	1:B:1173:LEU:HD23	1.68	0.75
1:C:1234:PRO:HB2	1:C:1237:CYS:HB2	1.70	0.74
1:C:1104:LEU:HD23	3:C:306:SO4:O2	1.89	0.73
1:C:1074:PRO:O	1:C:1076:LEU:HG	1.88	0.72
1:A:1003:ARG:HG3	1:A:1003:ARG:NH1	2.03	0.72
1:B:1074:PRO:O	1:B:1076:LEU:HG	1.90	0.72
1:A:1234:PRO:HB2	1:A:1237:CYS:HB2	1.72	0.72
1:C:995:ALA:HB1	1:C:997:GLU:OE2	1.90	0.71
1:C:1092:ARG:NH2	1:C:1095:ARG:NE	2.32	0.71
1:C:1053:VAL:HG11	1:C:1156:MET:HG3	1.73	0.71
1:A:1074:PRO:O	1:A:1076:LEU:HG	1.90	0.70
1:A:995:ALA:HB1	1:A:997:GLU:OE2	1.90	0.70
1:A:1092:ARG:HH21	1:A:1095:ARG:HE	1.39	0.70
1:B:1073:GLN:HB3	1:B:1074:PRO:HD2	1.74	0.70
1:B:1003:ARG:HG3	1:B:1003:ARG:NH1	2.03	0.70
1:B:995:ALA:HB1	1:B:997:GLU:OE2	1.92	0.69
1:C:1053:VAL:CG1	1:C:1156:MET:CE	2.66	0.69
1:B:1106:PRO:O	1:B:1107:PRO:O	2.10	0.69
1:C:1040:SER:O	1:C:1044:ARG:HG3	1.93	0.68
1:B:1145:GLU:OE2	1:B:1145:GLU:HA	1.95	0.67
1:B:1040:SER:O	1:B:1044:ARG:HG3	1.95	0.66
1:B:1114:GLN:O	1:B:1118:GLU:HG3	1.95	0.66
1:C:1053:VAL:CG1	1:C:1156:MET:HE2	2.21	0.66
1:C:1145:GLU:HA	1:C:1145:GLU:OE2	1.97	0.65
1:A:1207:THR:HB	1:A:1210:GLU:HG3	1.78	0.65
1:A:1045:ILE:HG12	1:B:1173:LEU:HD21	1.79	0.64
1:B:1239:ASP:O	1:B:1243:GLU:HG2	1.98	0.64
1:C:1239:ASP:O	1:C:1243:GLU:HG2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1040:SER:O	1:A:1044:ARG:HG3	1.96	0.64
1:C:1114:GLN:O	1:C:1118:GLU:HG3	1.96	0.64
1:B:1207:THR:HB	1:B:1210:GLU:HG3	1.79	0.63
1:A:1045:ILE:HG12	1:B:1173:LEU:CD2	2.29	0.62
1:A:1145:GLU:HA	1:A:1145:GLU:OE2	1.99	0.62
1:A:1114:GLN:O	1:A:1118:GLU:HG3	1.99	0.62
1:A:1078:ILE:HD12	1:A:1078:ILE:N	2.15	0.61
1:C:1167:ARG:HH11	1:C:1167:ARG:CB	2.14	0.61
1:C:1207:THR:HB	1:C:1210:GLU:HG3	1.82	0.61
1:C:1078:ILE:HD12	1:C:1078:ILE:N	2.16	0.60
1:A:1045:ILE:HD11	1:B:1172:GLY:HA2	1.82	0.60
1:C:1171:LYS:O	1:C:1171:LYS:HG3	2.01	0.60
1:C:1050:GLU:O	1:C:1053:VAL:CG2	2.48	0.59
1:A:1156:MET:O	1:A:1157:THR:HB	2.02	0.59
1:B:1078:ILE:N	1:B:1078:ILE:HD12	2.17	0.59
1:C:1092:ARG:NH2	1:C:1095:ARG:HE	1.95	0.59
1:C:1003:ARG:HG3	1:C:1003:ARG:NH1	2.17	0.59
1:A:1239:ASP:O	1:A:1243:GLU:HG2	2.02	0.59
1:B:1198:PHE:O	1:B:1201:VAL:HG22	2.03	0.58
1:A:1157:THR:HG21	1:C:984:ALA:N	2.18	0.58
1:A:1109:LEU:O	1:A:1113:ILE:HG12	2.04	0.58
1:C:1056:GLU:OE1	1:C:1167:ARG:NH2	2.36	0.58
1:C:1198:PHE:O	1:C:1201:VAL:HG22	2.04	0.57
1:A:1134:ARG:HD3	1:A:1168:LYS:HD2	1.86	0.57
1:C:1123:MET:HG2	1:C:1151:ILE:HD11	1.87	0.57
1:C:1007:GLN:HE22	1:C:1011:GLY:HA2	1.69	0.57
1:B:1082:MET:HE3	1:B:1144:ALA:N	2.20	0.57
1:C:1030:VAL:HG23	1:C:1032:ILE:HD11	1.86	0.57
1:B:1175:PRO:HG3	5:B:54:HOH:O	2.05	0.56
1:B:1030:VAL:HG23	1:B:1032:ILE:HD11	1.86	0.56
1:B:1109:LEU:O	1:B:1113:ILE:HG12	2.04	0.56
1:A:1030:VAL:HG23	1:A:1032:ILE:HD11	1.86	0.56
1:A:1045:ILE:CD1	1:B:1172:GLY:HA2	2.35	0.56
1:B:1123:MET:HG2	1:B:1151:ILE:HD11	1.87	0.56
1:A:1045:ILE:HG22	5:A:221:HOH:O	2.07	0.55
1:B:1167:ARG:HH11	1:B:1167:ARG:HG2	1.71	0.55
1:B:1275:ARG:HA	1:B:1281:TYR:CD1	2.41	0.55
1:B:1090:TYR:O	1:B:1093:SER:OG	2.25	0.55
1:C:1095:ARG:O	1:C:1097:GLU:N	2.37	0.55
1:A:988:VAL:HG22	1:B:1174:LEU:HD12	1.89	0.54
1:B:1073:GLN:CB	1:B:1074:PRO:HD2	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1257:PRO:HG2	1:B:1262:ILE:HD11	1.89	0.54
1:A:1123:MET:HG2	1:A:1151:ILE:HD11	1.90	0.54
1:B:1134:ARG:HD3	1:B:1168:LYS:HD2	1.89	0.54
1:B:985:ASP:OD1	1:B:985:ASP:N	2.40	0.54
1:A:1104:LEU:H	1:A:1104:LEU:HD22	1.67	0.54
1:A:1257:PRO:HG2	1:A:1262:ILE:HD11	1.90	0.54
1:A:1198:PHE:O	1:A:1201:VAL:HG22	2.08	0.54
1:C:1109:LEU:O	1:C:1113:ILE:HG12	2.08	0.54
1:C:1275:ARG:HA	1:C:1281:TYR:CD1	2.43	0.54
1:A:1112:MET:HE2	1:A:1206:ALA:HA	1.91	0.53
1:B:1003:ARG:NH1	1:B:1003:ARG:CG	2.68	0.53
1:B:1073:GLN:HB3	1:B:1074:PRO:CD	2.38	0.53
1:A:1139:ARG:HG3	1:A:1139:ARG:HH11	1.74	0.53
1:A:987:TYR:HB3	1:B:1173:LEU:CD2	2.36	0.53
1:C:1056:GLU:OE2	1:C:1167:ARG:NH2	2.42	0.53
1:A:1104:LEU:N	1:A:1104:LEU:CD2	2.68	0.52
1:B:1045:ILE:HD11	1:C:1172:GLY:CA	2.34	0.52
1:A:1275:ARG:HA	1:A:1281:TYR:CD1	2.44	0.52
1:C:1007:GLN:NE2	1:C:1011:GLY:HA2	2.23	0.52
1:C:1134:ARG:HD3	1:C:1168:LYS:HD2	1.90	0.52
1:B:1165:TYR:HE1	1:B:1168:LYS:HZ1	1.55	0.52
1:C:1252:ASN:O	1:C:1255:MET:HB2	2.10	0.52
1:C:1123:MET:SD	1:C:1151:ILE:HD13	2.51	0.51
1:C:1250:GLN:CB	1:C:1255:MET:HB3	2.41	0.51
1:A:1193:SER:HB2	5:A:151:HOH:O	2.10	0.51
1:A:1201:VAL:O	1:A:1205:ILE:HG13	2.10	0.50
1:B:1092:ARG:NH2	1:B:1095:ARG:CZ	2.71	0.50
1:C:1257:PRO:HG2	1:C:1262:ILE:HD11	1.93	0.50
1:A:1195:VAL:O	1:A:1198:PHE:HB3	2.12	0.50
1:C:1092:ARG:HE	1:C:1095:ARG:HE	1.58	0.50
1:A:1123:MET:SD	1:A:1151:ILE:HD13	2.52	0.49
1:C:1112:MET:HE2	1:C:1206:ALA:HA	1.94	0.49
1:C:1053:VAL:CG1	1:C:1156:MET:HE3	2.33	0.49
1:C:1113:ILE:HD11	1:C:1240:MET:SD	2.51	0.49
1:B:1113:ILE:HD11	1:B:1240:MET:SD	2.53	0.49
1:B:1184:LEU:HD22	1:B:1222:LEU:CD2	2.41	0.49
1:B:1004:GLU:HG2	1:B:1014:TYR:CE1	2.46	0.49
1:B:1036:ASN:OD1	1:B:1037:GLU:HG2	2.13	0.49
1:C:1139:ARG:HH11	1:C:1139:ARG:HG2	1.78	0.49
1:A:1004:GLU:HG2	1:A:1014:TYR:CE1	2.48	0.48
1:B:1258:SER:O	1:B:1262:ILE:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1134:ARG:NE	1:A:1168:LYS:HB3	2.28	0.48
1:C:1008:GLY:CA	4:C:303:ANP:O2B	2.62	0.48
1:C:1036:ASN:OD1	1:C:1037:GLU:HG2	2.13	0.48
1:A:1083:THR:OG1	1:A:1145:GLU:OE2	2.25	0.48
1:B:1123:MET:SD	1:B:1151:ILE:HD13	2.53	0.48
1:B:1260:LEU:HD11	1:B:1286:LYS:NZ	2.28	0.48
1:C:1019:LYS:HG2	1:C:1027:GLU:HG2	1.96	0.47
1:A:1053:VAL:HG12	1:A:1057:PHE:HE2	1.78	0.47
1:A:1173:LEU:HG	1:C:1041:MET:CE	2.44	0.47
1:B:1106:PRO:HB2	1:B:1107:PRO:HD2	1.96	0.47
1:A:1092:ARG:HH21	1:A:1095:ARG:NE	2.09	0.47
1:A:1133:HIS:O	1:A:1134:ARG:HB2	2.14	0.47
1:A:1184:LEU:HD22	1:A:1222:LEU:CD2	2.43	0.47
1:B:1019:LYS:HG2	1:B:1027:GLU:HG2	1.96	0.47
1:A:1113:ILE:HD11	1:A:1240:MET:SD	2.54	0.47
1:B:1113:ILE:HG23	1:B:1266:ILE:CG1	2.45	0.47
1:B:1130:LYS:HA	1:B:1166:TYR:CD1	2.50	0.47
1:C:1184:LEU:HD22	1:C:1222:LEU:CD2	2.39	0.47
1:C:1201:VAL:O	1:C:1205:ILE:HG13	2.14	0.47
1:C:1004:GLU:HG2	1:C:1014:TYR:CE1	2.50	0.47
1:A:1173:LEU:HG	1:C:1041:MET:HE1	1.96	0.47
1:C:1056:GLU:CD	1:C:1167:ARG:HH22	2.18	0.47
1:A:1258:SER:O	1:A:1262:ILE:HG12	2.14	0.47
1:A:1053:VAL:HA	5:A:235:HOH:O	2.15	0.47
1:C:1195:VAL:O	1:C:1198:PHE:HB3	2.15	0.47
1:A:1046:GLU:HA	5:A:221:HOH:O	2.14	0.46
1:A:1139:ARG:HH12	1:A:1140:ASN:HD21	1.62	0.46
1:C:1073:GLN:HB3	1:C:1074:PRO:HD2	1.72	0.46
1:B:1195:VAL:O	1:B:1198:PHE:HB3	2.15	0.46
1:C:1034:THR:HG22	1:C:1076:LEU:CD2	2.46	0.46
1:B:1167:ARG:HG2	1:B:1167:ARG:NH1	2.30	0.46
1:C:1035:VAL:HG12	1:C:1039:ALA:CB	2.45	0.46
1:A:1036:ASN:OD1	1:A:1037:GLU:HG2	2.15	0.46
1:B:1095:ARG:NH2	1:B:1210:GLU:HG2	2.30	0.46
1:A:1081:LEU:HD13	1:A:1083:THR:HG23	1.98	0.46
1:B:1259:PHE:O	1:B:1263:ILE:HG13	2.16	0.46
1:C:1133:HIS:O	1:C:1134:ARG:HB2	2.16	0.46
1:C:1056:GLU:CD	1:C:1167:ARG:NH2	2.70	0.46
1:B:1112:MET:HE2	1:B:1205:ILE:HG22	1.98	0.46
1:A:1113:ILE:HD11	1:A:1240:MET:HE1	1.97	0.45
1:B:1211:GLN:O	1:B:1214:GLN:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1019:LYS:HG2	1:A:1027:GLU:HG2	1.98	0.45
1:A:1035:VAL:HG12	1:A:1039:ALA:CB	2.47	0.45
1:A:1113:ILE:HD11	1:A:1240:MET:CE	2.47	0.45
1:A:1211:GLN:O	1:A:1214:GLN:HB2	2.17	0.45
1:A:1078:ILE:N	1:A:1078:ILE:CD1	2.79	0.45
1:C:1019:LYS:HE3	1:C:1027:GLU:CG	2.46	0.45
1:C:1211:GLN:O	1:C:1214:GLN:HB2	2.17	0.45
1:B:1217:SER:OG	1:B:1220:GLN:HG3	2.17	0.45
1:C:1078:ILE:CD1	1:C:1078:ILE:N	2.80	0.45
1:B:1082:MET:HE3	1:B:1143:VAL:C	2.37	0.45
1:B:1286:LYS:HD2	1:B:1286:LYS:H	1.82	0.45
1:C:1113:ILE:HD11	1:C:1240:MET:HE1	1.99	0.45
1:C:1250:GLN:HB3	1:C:1255:MET:HB3	1.97	0.45
1:C:1258:SER:O	1:C:1262:ILE:HG12	2.17	0.45
1:A:1167:ARG:HH11	1:A:1167:ARG:HG2	1.83	0.44
1:A:1217:SER:OG	1:A:1220:GLN:HG3	2.18	0.44
1:C:1217:SER:OG	1:C:1220:GLN:HG3	2.18	0.44
1:A:1034:THR:HG22	1:A:1076:LEU:CD2	2.47	0.44
1:B:1113:ILE:HD11	1:B:1240:MET:CE	2.47	0.44
1:B:1084:ARG:HG2	1:B:1084:ARG:HH11	1.82	0.44
1:C:1081:LEU:HD13	1:C:1083:THR:HG23	1.99	0.44
1:A:1139:ARG:NH1	1:A:1140:ASN:ND2	2.65	0.44
1:B:1030:VAL:HG23	1:B:1032:ILE:CD1	2.47	0.44
1:B:1035:VAL:HG12	1:B:1039:ALA:CB	2.47	0.44
1:B:1033:LYS:NZ	4:B:302:ANP:O1B	2.45	0.44
1:C:1030:VAL:HG23	1:C:1032:ILE:CD1	2.47	0.44
1:A:1095:ARG:HH22	1:A:1210:GLU:CG	2.21	0.44
1:B:1139:ARG:NH1	1:B:1140:ASN:OD1	2.51	0.44
1:B:1250:GLN:HB3	1:B:1255:MET:HB3	2.00	0.44
1:C:1135:ASP:O	1:C:1140:ASN:ND2	2.51	0.44
1:C:1083:THR:OG1	1:C:1145:GLU:OE2	2.26	0.43
1:C:1113:ILE:HD11	1:C:1240:MET:CE	2.47	0.43
1:B:1106:PRO:CB	1:B:1107:PRO:HD2	2.49	0.43
1:B:1175:PRO:HG2	5:B:182:HOH:O	2.18	0.43
1:B:1078:ILE:N	1:B:1078:ILE:CD1	2.82	0.43
1:C:1066:LEU:HB2	1:C:1078:ILE:HG22	1.99	0.43
1:A:1030:VAL:HG23	1:A:1032:ILE:CD1	2.48	0.43
1:C:1007:GLN:HA	1:C:1012:MET:HA	2.00	0.43
1:A:1019:LYS:HE3	1:A:1027:GLU:CG	2.49	0.43
1:B:1036:ASN:OD1	1:B:1037:GLU:N	2.52	0.43
1:B:1113:ILE:HG23	1:B:1266:ILE:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1107:PRO:HB2	1:C:1112:MET:HE3	2.01	0.43
1:B:1034:THR:HG22	1:B:1076:LEU:CD2	2.49	0.42
1:B:1201:VAL:O	1:B:1205:ILE:HG13	2.18	0.42
1:A:1084:ARG:HG2	1:A:1084:ARG:HH11	1.83	0.42
1:A:1236:ASN:HB2	5:A:227:HOH:O	2.18	0.42
1:B:1081:LEU:HD13	1:B:1083:THR:HG23	2.00	0.42
1:A:1156:MET:O	1:A:1157:THR:CB	2.67	0.42
1:B:1108:SER:OG	1:B:1111:LYS:HG2	2.19	0.42
1:B:1082:MET:HE1	1:B:1144:ALA:HB2	2.00	0.42
1:B:1113:ILE:HD11	1:B:1240:MET:HE1	2.02	0.42
1:A:1259:PHE:O	1:A:1263:ILE:HG13	2.20	0.42
1:C:1095:ARG:HH22	1:C:1210:GLU:HG2	1.84	0.42
1:A:1108:SER:OG	1:A:1111:LYS:HG2	2.20	0.42
1:A:1139:ARG:HG3	1:A:1139:ARG:NH1	2.35	0.41
1:C:1259:PHE:O	1:C:1263:ILE:HG13	2.20	0.41
1:A:1139:ARG:HH12	1:A:1140:ASN:ND2	2.19	0.41
1:C:1092:ARG:NE	1:C:1095:ARG:HE	2.18	0.41
1:B:1007:GLN:NE2	1:B:1011:GLY:HA2	2.34	0.41
1:A:1135:ASP:O	1:A:1140:ASN:ND2	2.52	0.41
1:A:1131:PHE:CD2	1:A:1156:MET:HE2	2.56	0.41
1:B:1019:LYS:HE3	1:B:1027:GLU:CG	2.50	0.41
1:A:1073:GLN:HB3	1:A:1074:PRO:HD2	1.80	0.41
1:A:986:VAL:CG2	1:B:1172:GLY:O	2.60	0.41
1:C:1084:ARG:HH11	1:C:1084:ARG:HG2	1.85	0.41
1:C:1243:GLU:HA	1:C:1243:GLU:OE2	2.21	0.41
1:B:1156:MET:HB2	1:B:1156:MET:HE3	1.80	0.41
1:B:1243:GLU:OE2	1:B:1243:GLU:HA	2.21	0.41
1:C:1036:ASN:OD1	1:C:1037:GLU:N	2.54	0.40
1:C:1131:PHE:HE2	1:C:1156:MET:HG2	1.86	0.40
1:A:1171:LYS:NZ	5:A:249:HOH:O	2.54	0.40
1:B:1133:HIS:O	1:B:1134:ARG:HB2	2.21	0.40
1:C:1037:GLU:HG3	1:C:1038:ALA:N	2.36	0.40
1:B:1285:ASN:OD1	1:B:1286:LYS:HD3	2.21	0.40
1:C:1250:GLN:HG3	1:C:1255:MET:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	285/308 (92%)	273 (96%)	11 (4%)	1 (0%)	38	35
1	B	281/308 (91%)	268 (95%)	11 (4%)	2 (1%)	25	20
1	C	285/308 (92%)	273 (96%)	9 (3%)	3 (1%)	17	11
All	All	851/924 (92%)	814 (96%)	31 (4%)	6 (1%)	25	20

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1074	PRO
1	B	1074	PRO
1	B	1107	PRO
1	C	1074	PRO
1	C	985	ASP
1	C	1096	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	253/268 (94%)	242 (96%)	11 (4%)	33	32
1	B	250/268 (93%)	239 (96%)	11 (4%)	33	31
1	C	253/268 (94%)	239 (94%)	14 (6%)	25	22
All	All	756/804 (94%)	720 (95%)	36 (5%)	30	27

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	994	VAL
1	A	1003	ARG
1	A	1048	LEU
1	A	1074	PRO
1	A	1081	LEU
1	A	1093	SER
1	A	1109	LEU
1	A	1157	THR
1	A	1165	TYR
1	A	1191	THR
1	A	1268	GLU
1	B	985	ASP
1	B	1003	ARG
1	B	1048	LEU
1	B	1074	PRO
1	B	1081	LEU
1	B	1109	LEU
1	B	1167	ARG
1	B	1191	THR
1	B	1222	LEU
1	B	1255	MET
1	B	1268	GLU
1	C	994	VAL
1	C	1003	ARG
1	C	1048	LEU
1	C	1053	VAL
1	C	1074	PRO
1	C	1081	LEU
1	C	1103	VAL
1	C	1109	LEU
1	C	1157	THR
1	C	1166	TYR
1	C	1167	ARG
1	C	1191	THR
1	C	1255	MET
1	C	1268	GLU

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	1214	GLN

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Mol	Chain	Res	Type
1	B	1007	GLN
1	B	1214	GLN
1	C	1007	GLN
1	C	1071	GLN
1	C	1214	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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	$\# Z > 2$
4	ANP	A	301	2	29,33,33	2.61	9 (31%)	28,52,52	2.83	6 (21%)
3	SO4	A	305	1	4,4,4	0.41	0	6,6,6	0.12	0
4	ANP	B	302	-	29,33,33	2.32	8 (27%)	28,52,52	2.67	7 (25%)
3	SO4	B	307	-	4,4,4	0.21	0	6,6,6	0.08	0
4	ANP	C	303	-	29,33,33	2.28	9 (31%)	28,52,52	2.60	7 (25%)
3	SO4	C	306	-	4,4,4	0.49	0	6,6,6	0.12	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
4	ANP	A	301	2	-	0/13/38/38	0/3/3/3
3	SO4	A	305	1	-	0/0/0/0	0/0/0/0
4	ANP	B	302	-	-	0/13/38/38	0/3/3/3
3	SO4	B	307	-	-	0/0/0/0	0/0/0/0
4	ANP	C	303	-	-	0/13/38/38	0/3/3/3
3	SO4	C	306	-	-	0/0/0/0	0/0/0/0

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	303	ANP	PB-O2B	-5.10	1.42	1.56
4	A	301	ANP	PB-O2B	-4.49	1.44	1.56
4	A	301	ANP	C2'-C1'	-4.47	1.46	1.53
4	B	302	ANP	PB-O2B	-4.08	1.45	1.56
4	B	302	ANP	C2'-C1'	-3.68	1.47	1.53
4	C	303	ANP	C2'-C1'	-3.53	1.48	1.53
4	A	301	ANP	PG-O2G	-2.35	1.50	1.56
4	C	303	ANP	PG-O2G	-2.01	1.51	1.56
4	A	301	ANP	C5'-C4'	2.07	1.58	1.51
4	B	302	ANP	C2-N3	2.07	1.35	1.32
4	A	301	ANP	C2-N3	2.16	1.35	1.32
4	C	303	ANP	C2-N1	2.35	1.38	1.33
4	B	302	ANP	C2-N1	2.56	1.38	1.33
4	C	303	ANP	PG-N3B	2.61	1.70	1.63
4	A	301	ANP	PG-N3B	2.62	1.70	1.63
4	C	303	ANP	C2-N3	2.68	1.36	1.32
4	C	303	ANP	PB-O1B	3.29	1.49	1.46
4	B	302	ANP	PG-N3B	3.40	1.72	1.63
4	B	302	ANP	PB-O1B	3.76	1.50	1.46
4	A	301	ANP	PB-O3A	4.75	1.65	1.59
4	C	303	ANP	PG-O1G	4.91	1.51	1.46
4	B	302	ANP	PG-O1G	5.59	1.52	1.46
4	A	301	ANP	PG-O1G	5.84	1.52	1.46
4	C	303	ANP	PB-O3A	5.99	1.66	1.59
4	B	302	ANP	PB-O3A	6.18	1.66	1.59
4	A	301	ANP	PB-O1B	7.34	1.54	1.46

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	301	ANP	O1B-PB-N3B	-8.63	98.88	111.79
4	B	302	ANP	O1B-PB-N3B	-6.06	102.73	111.79
4	B	302	ANP	N3-C2-N1	-6.03	123.61	128.86
4	A	301	ANP	N3-C2-N1	-5.65	123.94	128.86
4	C	303	ANP	N3-C2-N1	-5.50	124.07	128.86
4	C	303	ANP	O1B-PB-N3B	-4.87	104.51	111.79
4	C	303	ANP	O1G-PG-N3B	-4.44	105.14	111.79
4	B	302	ANP	O1G-PG-N3B	-4.27	105.40	111.79
4	A	301	ANP	O1G-PG-N3B	-4.04	105.75	111.79
4	B	302	ANP	O4'-C4'-C3'	-3.03	99.14	105.17
4	A	301	ANP	O4'-C4'-C3'	-2.66	99.88	105.17
4	C	303	ANP	O4'-C4'-C3'	-2.56	100.07	105.17
4	C	303	ANP	O2'-C2'-C3'	2.00	118.24	111.83
4	B	302	ANP	O2'-C2'-C3'	2.06	118.42	111.83
4	A	301	ANP	O3A-PB-N3B	2.81	114.39	106.59
4	C	303	ANP	O3A-PB-N3B	3.27	115.67	106.59
4	B	302	ANP	O3A-PB-N3B	3.30	115.74	106.59
4	B	302	ANP	C4'-O4'-C1'	7.92	118.19	109.77
4	A	301	ANP	C4'-O4'-C1'	8.08	118.37	109.77
4	C	303	ANP	C4'-O4'-C1'	8.67	119.00	109.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	302	ANP	1	0
4	C	303	ANP	1	0
3	C	306	SO4	1	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	291/308 (94%)	0.36	14 (4%) 31 37	24, 42, 66, 84	0
1	B	287/308 (93%)	0.30	12 (4%) 37 44	24, 40, 65, 85	0
1	C	291/308 (94%)	0.40	15 (5%) 28 34	22, 39, 66, 83	0
All	All	869/924 (94%)	0.35	41 (4%) 32 38	22, 41, 66, 85	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	984	ALA	6.7
1	C	1286	LYS	6.0
1	A	1157	THR	5.9
1	B	1286	LYS	4.9
1	C	984	ALA	4.8
1	C	1165	TYR	4.7
1	C	1042	ARG	4.5
1	C	1038	ALA	4.3
1	C	1039	ALA	3.9
1	C	1036	ASN	3.6
1	A	1165	TYR	3.6
1	A	1096	PRO	3.3
1	C	1171	LYS	3.3
1	C	1019	LYS	3.2
1	A	1042	ARG	2.9
1	B	1165	TYR	2.9
1	A	1216	LEU	2.7
1	B	1074	PRO	2.7
1	B	1109	LEU	2.7
1	B	1042	ARG	2.6
1	B	1107	PRO	2.5
1	A	1235	ASP	2.5
1	C	1076	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1218	ASN	2.5
1	B	984	ALA	2.4
1	B	1096	PRO	2.4
1	A	1173	LEU	2.4
1	A	1223	ARG	2.3
1	B	1106	PRO	2.3
1	C	1073	GLN	2.3
1	A	1097	GLU	2.2
1	B	1283	GLU	2.2
1	C	1027	GLU	2.2
1	B	1171	LYS	2.2
1	C	985	ASP	2.1
1	A	1038	ALA	2.1
1	C	1043	GLU	2.1
1	B	1235	ASP	2.1
1	A	1269	GLU	2.0
1	A	1246	ARG	2.0
1	C	1156	MET	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	SO4	A	305	5/5	0.95	0.22	3.81	20,20,20,20	5
3	SO4	C	306	5/5	0.89	0.18	1.19	20,20,20,20	5
4	ANP	C	303	31/31	0.90	0.15	0.11	45,54,72,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	SO4	B	307	5/5	0.93	0.13	-0.16	19,19,19,19	5
4	ANP	B	302	31/31	0.92	0.13	-0.19	28,46,76,79	0
4	ANP	A	301	31/31	0.94	0.12	-0.25	39,53,71,72	0
2	MG	A	304	1/1	0.96	0.07	-	54,54,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.