



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:22 PM UTC

PDB ID : 8V5F / pdb_00008v5f
Title : Nan Regulatory Protein Full-length from Streptococcus pneumoniae
Authors : Wood, D.M.; Dobson, R.C.J.; Horne, C.R.
Deposited on : 2023-11-30
Resolution : 2.55 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

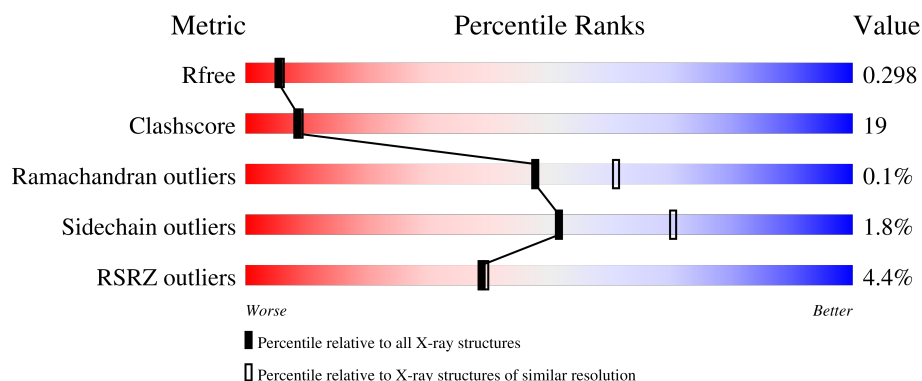
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	283	 4% 62% 31% 6%
1	B	283	 4% 57% 36% 7%
1	C	283	 2% 43% 20% 35%
1	D	283	 5% 60% 32% 6%

2 Entry composition [i](#)

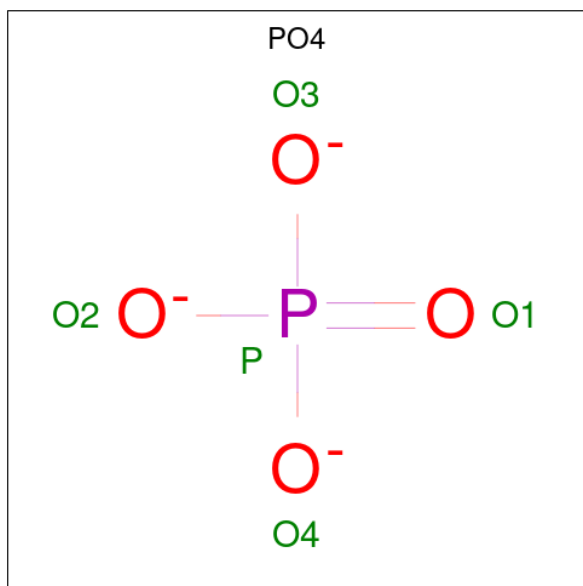
There are 5 unique types of molecules in this entry. The entry contains 15655 atoms, of which 7707 are hydrogens and 0 are deuteriums.

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 Phosphosugar-binding transcriptional regulator.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	266	Total	C	H	N	O	S	0	0	0
			4234	1356	2094	356	418	10			
1	B	264	Total	C	H	N	O	S	0	0	0
			4185	1341	2066	353	415	10			
1	C	184	Total	C	H	N	O	S	0	0	0
			2933	936	1463	243	283	8			
1	D	265	Total	C	H	N	O	S	0	0	0
			4218	1351	2084	355	418	10			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



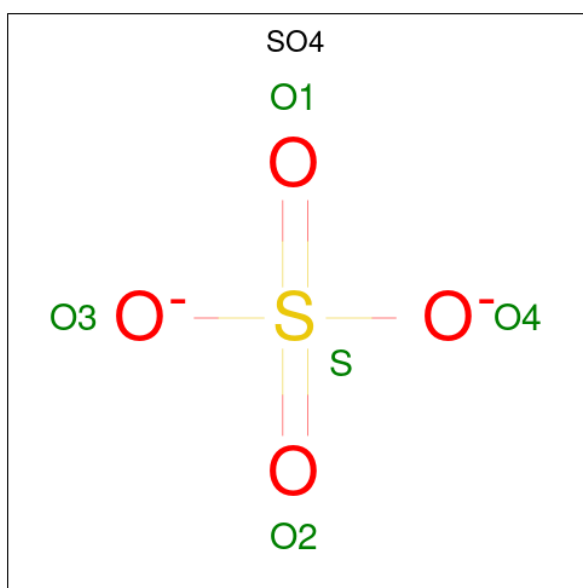
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		

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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



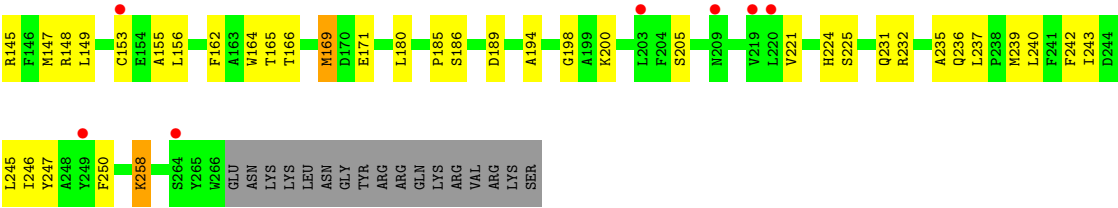
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

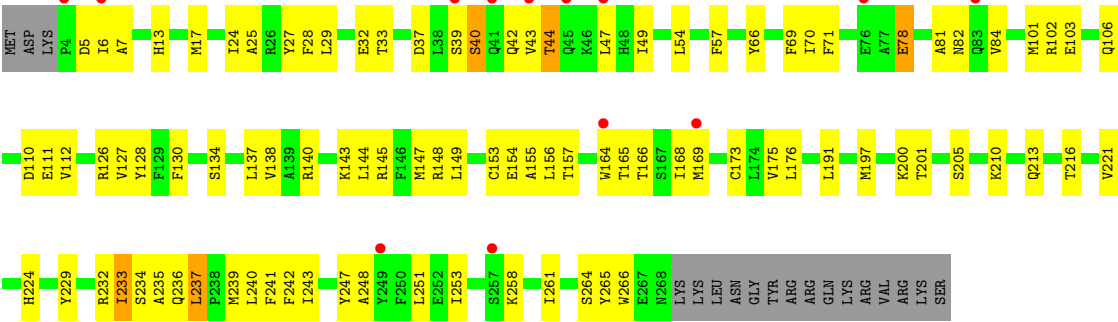
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Cl 1	0	0
4	B	1	Total 1	Cl 1	0	0
4	C	1	Total 1	Cl 1	0	0
4	D	1	Total 1	Cl 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	9	Total 9	O 9	0	0
5	B	7	Total 7	O 7	0	0
5	C	4	Total 4	O 4	0	0
5	D	1	Total 1	O 1	0	0



● Molecule 1: Phosphosugar-binding transcriptional regulator



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	53.24Å 109.23Å 202.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.91 – 2.55 45.91 – 2.55	Depositor EDS
% Data completeness (in resolution range)	97.7 (45.91-2.55) 97.6 (45.91-2.55)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.54Å)	Xtriage
Refinement program	REFMAC 8.0.013, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.262 , 0.313 (Not available) , 0.298	Depositor DCC
R_{free} test set	1903 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	54.1	Xtriage
Anisotropy	0.684	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15655	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% 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: CL, PO4, 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	0.25	0/2180	0.45	0/2945
1	B	0.32	0/2158	0.50	1/2917 (0.0%)
1	C	0.28	0/1497	0.44	1/2023 (0.0%)
1	D	0.30	0/2174	0.51	1/2937 (0.0%)
All	All	0.29	0/8009	0.48	3/10822 (0.0%)

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	B	0	1
1	C	0	1
1	D	0	2
All	All	0	4

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	185	PRO	N-CD-CG	-7.39	92.11	103.20
1	D	44	THR	N-CA-C	-6.47	103.73	111.69
1	C	86	LYS	CD-CE-NZ	-5.20	95.27	111.90

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	140	ARG	Sidechain
1	C	96	ARG	Sidechain
1	D	102	ARG	Sidechain
1	D	145	ARG	Sidechain

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	2140	2094	2092	83	2
1	B	2119	2066	2061	107	0
1	C	1470	1463	1463	47	0
1	D	2134	2084	2084	82	3
2	A	15	0	0	1	1
2	B	10	0	0	1	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	5	0	0	1	0
3	B	10	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	A	1	0	0	1	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	1	0
5	A	9	0	0	0	0
5	B	7	0	0	0	0
5	C	4	0	0	0	0
5	D	1	0	0	0	0
All	All	7948	7707	7700	297	3

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 19.

All (297) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:PHE:O	1:A:166:THR:HG23	1.75	0.87
1:B:143:LYS:NZ	1:B:147:MET:SD	2.48	0.87
1:B:159:GLN:N	1:B:159:GLN:OE1	2.08	0.86
1:A:216:THR:HG22	1:A:217:GLU:HG2	1.55	0.86
1:D:24:ILE:HD11	1:D:49:ILE:HD13	1.58	0.85
1:B:162:PHE:O	1:B:166:THR:HG23	1.76	0.84
1:A:138:VAL:HG23	1:A:236:GLN:HG2	1.61	0.82
1:A:130:PHE:CE1	1:A:156:LEU:HD12	2.16	0.80
1:B:176:LEU:HD23	1:B:202:VAL:HB	1.64	0.79
1:C:156:LEU:HD11	1:C:165:THR:HG21	1.64	0.79
1:D:156:LEU:HD21	1:D:165:THR:HG21	1.66	0.78
1:B:81:ALA:HA	1:B:84:VAL:HG12	1.66	0.76
1:C:166:THR:HA	1:C:169:MET:HE2	1.68	0.76
1:B:156:LEU:HD21	1:B:165:THR:HG21	1.69	0.75
1:C:137:LEU:HD21	1:D:140:ARG:HB2	1.67	0.74
1:A:237:LEU:HD23	1:A:240:LEU:HD12	1.70	0.74
1:B:108:LEU:HD22	1:B:220:LEU:HD22	1.68	0.74
1:A:101:MET:HE1	1:A:237:LEU:HB2	1.68	0.74
1:A:86:LYS:H	1:A:86:LYS:HD3	1.53	0.74
1:A:32:GLU:OE1	1:A:32:GLU:N	2.18	0.73
1:C:180:LEU:HG	1:C:239:MET:HE2	1.72	0.72
1:B:140:ARG:O	1:B:144:LEU:HD12	1.91	0.70
1:D:81:ALA:HB1	1:D:84:VAL:HG12	1.75	0.69
1:A:134:SER:HA	1:A:137:LEU:HD13	1.76	0.68
1:A:188:LEU:HD13	1:A:215:TYR:OH	1.94	0.67
1:C:221:VAL:HG12	1:C:242:PHE:CD2	2.29	0.67
1:C:145:ARG:NH1	1:D:233:ILE:O	2.27	0.67
1:B:84:VAL:HG22	1:B:85:SER:H	1.59	0.66
1:D:134:SER:HA	1:D:137:LEU:HD12	1.77	0.66
1:B:17:MET:HG2	1:B:21:GLU:HB2	1.76	0.65
1:B:27:TYR:CE2	1:B:33:THR:HG23	2.32	0.65
1:A:224:HIS:CB	1:A:232:ARG:HD3	2.27	0.64
1:D:27:TYR:CZ	1:D:33:THR:HG23	2.33	0.63
1:D:239:MET:O	1:D:243:ILE:HD13	1.98	0.63
1:A:157:THR:HG22	1:A:157:THR:O	1.98	0.63
1:B:155:ALA:C	1:B:156:LEU:HD12	2.23	0.63
1:C:155:ALA:O	1:C:156:LEU:HD23	1.99	0.63
1:A:261:ILE:O	1:A:264:SER:OG	2.16	0.62
1:D:251:LEU:HD12	1:D:251:LEU:O	1.98	0.62
1:D:234:SER:OG	1:D:235:ALA:N	2.31	0.62
1:C:87:HIS:HE1	1:D:106:GLN:HG3	1.66	0.61
1:A:230:ILE:HD12	1:A:230:ILE:H	1.63	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:ILE:HG12	1:D:47:LEU:HD13	1.83	0.61
1:A:224:HIS:HB2	1:A:232:ARG:HD3	1.82	0.60
1:B:108:LEU:CD2	1:B:220:LEU:HD22	2.32	0.60
1:C:90:LEU:HD12	1:D:248:ALA:HB1	1.83	0.60
1:A:142:MET:HE1	1:A:176:LEU:CD2	2.33	0.59
1:A:175:VAL:CG1	1:A:201:THR:HG22	2.33	0.59
1:A:10:ILE:HD11	1:A:69:PHE:HE1	1.68	0.58
1:A:144:LEU:O	1:A:148:ARG:HG3	2.02	0.58
1:A:90:LEU:HD11	1:B:252:GLU:HG3	1.86	0.58
1:A:54:LEU:HD21	1:A:66:TYR:CG	2.39	0.58
1:B:32:GLU:H	1:B:32:GLU:CD	2.12	0.58
1:D:157:THR:HG22	1:D:157:THR:O	2.03	0.57
1:C:180:LEU:HD11	1:C:235:ALA:O	2.03	0.57
1:C:240:LEU:HD23	1:D:237:LEU:CD2	2.34	0.57
1:C:88:SER:HB2	1:C:89:PRO:HD2	1.84	0.57
1:C:143:LYS:HD3	1:C:147:MET:HE3	1.86	0.57
1:B:221:VAL:HG12	1:B:242:PHE:CD1	2.39	0.57
1:D:224:HIS:HB3	1:D:232:ARG:HG2	1.85	0.57
1:B:207:VAL:HG13	1:B:208:PRO:HD2	1.86	0.57
1:D:221:VAL:HG12	1:D:242:PHE:CD2	2.40	0.56
1:B:253:ILE:HG22	1:B:254:ASN:OD1	2.04	0.56
1:A:10:ILE:HG21	1:A:29:LEU:CD1	2.36	0.56
1:A:49:ILE:HD11	1:A:54:LEU:HB2	1.88	0.55
1:A:133:GLY:O	1:A:137:LEU:HD12	2.06	0.55
1:A:175:VAL:HG13	1:A:201:THR:HG22	1.89	0.55
1:B:202:VAL:HG13	1:B:217:GLU:HB2	1.89	0.55
1:A:54:LEU:HD21	1:A:66:TYR:CD1	2.42	0.55
1:A:86:LYS:HD3	1:A:86:LYS:N	2.20	0.54
1:A:40:SER:O	1:A:44:THR:HG23	2.06	0.54
1:B:237:LEU:HA	1:B:240:LEU:HD12	1.89	0.54
1:D:40:SER:O	1:D:44:THR:HG23	2.07	0.54
1:B:180:LEU:N	2:B:301:PO4:O2	2.41	0.54
1:C:236:GLN:HB3	1:C:240:LEU:HD11	1.89	0.54
1:B:31:ALA:O	1:B:34:ILE:HG22	2.07	0.54
1:B:220:LEU:HD23	1:B:221:VAL:O	2.08	0.54
1:C:88:SER:N	1:D:111:GLU:OE2	2.36	0.54
1:D:39:SER:O	1:D:40:SER:CB	2.56	0.54
1:B:84:VAL:HG22	1:B:85:SER:N	2.23	0.54
1:B:209:ASN:HB3	1:B:212:SER:HB2	1.89	0.54
1:B:80:GLN:O	1:B:82:ASN:N	2.41	0.54
1:B:176:LEU:HD22	1:B:204:PHE:HE1	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:THR:HA	1:A:169:MET:HE2	1.89	0.53
1:D:166:THR:O	1:D:197:MET:HG3	2.09	0.53
1:D:49:ILE:HD11	1:D:54:LEU:HD13	1.91	0.52
1:A:158:ASP:OD1	1:A:160:ASP:N	2.43	0.52
1:A:32:GLU:H	1:A:32:GLU:CD	2.15	0.52
1:D:229:TYR:HA	1:D:232:ARG:HD2	1.90	0.52
1:B:176:LEU:HD22	1:B:204:PHE:CE1	2.44	0.52
1:A:106:GLN:HG3	1:B:87(C):HIS:NE2	2.24	0.52
1:D:253:ILE:O	1:D:258:LYS:HD2	2.10	0.52
1:B:17:MET:HG2	1:B:21:GLU:CB	2.40	0.52
1:A:86:LYS:HE2	1:A:87:HIS:CE1	2.45	0.51
3:A:304:SO4:O1	1:B:86:LYS:NZ	2.42	0.51
1:D:175:VAL:HG13	1:D:191:LEU:HD23	1.92	0.51
1:B:87(C):HIS:HB2	1:B:92:LYS:HE3	1.93	0.51
1:D:28:PHE:HE2	1:D:70:ILE:CD1	2.23	0.51
1:A:101:MET:HE1	1:A:237:LEU:CB	2.37	0.51
1:D:233:ILE:HG12	4:D:303:CL:CL	2.48	0.51
1:A:10:ILE:HB	1:A:29:LEU:HD11	1.92	0.51
1:A:111:GLU:OE1	1:A:249:TYR:OH	2.27	0.51
1:C:140:ARG:HB3	1:D:137:LEU:HD21	1.93	0.51
1:D:5:ASP:C	1:D:5:ASP:OD1	2.54	0.51
1:B:234:SER:HB3	1:B:237:LEU:HG	1.93	0.51
1:D:78:GLU:OE2	1:D:82:ASN:OD1	2.28	0.51
1:B:101:MET:HE1	1:B:237:LEU:CB	2.40	0.51
1:A:129:PHE:CE1	1:A:142:MET:HE2	2.45	0.50
1:A:156:LEU:HD11	1:A:165:THR:OG1	2.11	0.50
1:A:10:ILE:HD11	1:A:69:PHE:CE1	2.46	0.50
1:B:18:THR:O	1:B:22:GLN:HG3	2.12	0.50
1:D:71:PHE:CD1	1:D:71:PHE:C	2.90	0.50
1:B:203:LEU:HD12	1:B:204:PHE:N	2.27	0.50
2:A:301:PO4:O1	1:D:140:ARG:NH2	2.44	0.50
1:A:10:ILE:HG21	1:A:29:LEU:HD13	1.94	0.50
1:A:87:HIS:NE2	1:B:106:GLN:HG3	2.27	0.49
1:A:142:MET:HE1	1:A:176:LEU:HD22	1.93	0.49
1:C:114:LEU:HD23	1:C:245:LEU:HB3	1.94	0.49
1:D:24:ILE:CD1	1:D:49:ILE:HD13	2.35	0.49
1:B:101:MET:HE1	1:B:237:LEU:HB3	1.94	0.49
1:A:6:ILE:HD13	1:A:72:GLN:HB3	1.93	0.49
1:A:86:LYS:H	1:A:86:LYS:CD	2.25	0.49
1:B:210:LYS:HG3	1:B:210:LYS:O	2.13	0.49
1:A:125:GLU:HG2	1:A:172:ASN:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ILE:HG12	4:A:305:CL:CL	2.50	0.49
1:B:49:ILE:HD12	1:B:49:ILE:C	2.38	0.49
1:B:15:GLU:O	1:B:17:MET:N	2.45	0.49
1:B:81:ALA:HA	1:B:84:VAL:CG1	2.41	0.49
1:B:164:TRP:CZ3	1:D:144:LEU:HG	2.47	0.49
1:A:251:LEU:HG	1:A:255:ARG:HD2	1.94	0.49
1:B:221:VAL:HG12	1:B:242:PHE:CE1	2.48	0.49
1:B:144:LEU:HD23	1:D:164:TRP:HZ3	1.78	0.48
1:B:250:PHE:CE2	1:B:258:LYS:HE2	2.47	0.48
1:C:162:PHE:O	1:C:166:THR:HG23	2.13	0.48
1:B:127:VAL:O	1:B:153:CYS:HA	2.12	0.48
1:D:205:SER:C	1:D:221:VAL:HG22	2.38	0.48
1:B:144:LEU:HD12	1:B:144:LEU:H	1.77	0.48
1:A:164:TRP:HB3	1:C:147:MET:SD	2.53	0.48
1:D:130:PHE:HE1	1:D:156:LEU:HD13	1.78	0.48
1:B:110:ASP:OD1	1:B:112:VAL:HG12	2.13	0.48
1:D:128:TYR:CD2	1:D:169:MET:HE2	2.48	0.48
1:D:155:ALA:C	1:D:156:LEU:HD12	2.39	0.48
1:A:142:MET:HE1	1:A:176:LEU:HD23	1.96	0.47
1:B:44:THR:HG22	1:B:49:ILE:CD1	2.44	0.47
1:D:81:ALA:CB	1:D:84:VAL:HG12	2.44	0.47
1:A:10:ILE:HD13	1:A:61:CYS:SG	2.54	0.47
1:A:191:LEU:O	1:A:201:THR:HG21	2.13	0.47
1:A:138:VAL:HG13	1:A:243:ILE:CD1	2.44	0.47
1:B:141:GLU:HA	1:B:144:LEU:CD1	2.44	0.47
1:B:143:LYS:HD2	1:B:154:GLU:HA	1.96	0.47
1:C:117:ILE:HG21	1:C:246:ILE:HD13	1.95	0.47
1:C:138:VAL:HG13	1:C:243:ILE:CD1	2.44	0.47
1:C:185:PRO:O	1:C:189:ASP:OD1	2.32	0.47
1:A:81:ALA:O	1:A:84:VAL:HG22	2.15	0.47
1:C:149:LEU:HD11	1:C:247:TYR:CE2	2.49	0.47
1:D:43:VAL:HG11	1:D:66:TYR:OH	2.15	0.47
1:B:6:ILE:HD12	1:B:6:ILE:H	1.80	0.47
1:B:81:ALA:O	1:B:84:VAL:HG12	2.15	0.47
1:C:93:ARG:NH2	1:C:231:GLN:OE1	2.48	0.47
1:D:6:ILE:N	1:D:6:ILE:HD12	2.29	0.47
1:A:49:ILE:HG13	1:A:50:SER:O	2.15	0.47
1:A:211:ASP:N	1:A:211:ASP:OD1	2.45	0.47
1:B:14:PHE:HE1	1:B:22:GLN:CB	2.28	0.47
1:A:28:PHE:CE1	1:A:69:PHE:HE2	2.33	0.46
1:B:6:ILE:HD13	1:B:76:GLU:HG2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:GLN:HB3	1:C:240:LEU:CD1	2.45	0.46
1:D:265:TYR:C	1:D:265:TYR:CD2	2.94	0.46
1:B:20:LEU:HD11	1:B:49:ILE:CG2	2.45	0.46
1:B:81:ALA:CA	1:B:84:VAL:HG12	2.40	0.46
1:D:175:VAL:C	1:D:176:LEU:HD12	2.41	0.46
1:D:261:ILE:O	1:D:264:SER:OG	2.32	0.46
1:A:104:GLN:OE1	1:A:222:ALA:HA	2.15	0.46
1:A:98:TYR:CD2	1:B:241:PHE:CE1	3.03	0.46
1:A:110:ASP:O	1:A:114:LEU:HD13	2.16	0.46
1:B:122:GLU:OE1	1:B:258:LYS:NZ	2.49	0.46
1:D:54:LEU:HD21	1:D:66:TYR:CZ	2.51	0.46
1:C:109:ILE:HD11	1:C:245:LEU:HD11	1.98	0.46
1:C:236:GLN:C	1:C:240:LEU:HD13	2.41	0.46
1:D:144:LEU:O	1:D:148:ARG:HG3	2.16	0.46
1:B:44:THR:HG22	1:B:49:ILE:HD12	1.97	0.46
1:D:149:LEU:HD11	1:D:247:TYR:CE2	2.51	0.46
1:B:121:ILE:HD13	1:B:146:PHE:HE1	1.80	0.46
1:A:224:HIS:CG	1:A:232:ARG:HD3	2.50	0.46
1:B:142:MET:SD	1:B:243:ILE:HG12	2.56	0.46
1:B:101:MET:HE3	1:B:241:PHE:HE2	1.81	0.45
1:A:127:VAL:O	1:A:153:CYS:HA	2.16	0.45
1:B:38:LEU:HB3	1:B:70:ILE:HD11	1.97	0.45
1:B:203:LEU:HD22	1:B:215:TYR:HE2	1.79	0.45
1:D:43:VAL:HG21	1:D:54:LEU:HD21	1.98	0.45
1:B:200:LYS:HE2	1:B:200:LYS:HB2	1.72	0.45
1:B:223:THR:HG22	1:B:224:HIS:N	2.31	0.45
1:C:250:PHE:CE2	1:C:258:LYS:HE2	2.52	0.45
1:B:20:LEU:HD11	1:B:49:ILE:HG22	1.98	0.45
1:B:265:TYR:C	1:B:265:TYR:CD2	2.95	0.45
1:C:221:VAL:HA	1:C:242:PHE:CE2	2.51	0.45
1:B:14:PHE:HE1	1:B:22:GLN:HB3	1.80	0.45
1:B:27:TYR:HD1	1:B:47:LEU:HD22	1.81	0.45
1:D:32:GLU:OE1	1:D:32:GLU:N	2.28	0.45
1:C:138:VAL:HG23	1:C:236:GLN:HG2	1.98	0.45
1:A:142:MET:CE	1:A:176:LEU:HD22	2.47	0.45
1:B:30:GLN:HB3	1:B:32:GLU:OE2	2.15	0.45
1:D:37:ASP:HB3	1:D:42:GLN:HG2	1.99	0.45
1:D:126:ARG:NH1	1:D:173:CYS:SG	2.90	0.45
1:C:205:SER:C	1:C:221:VAL:HG22	2.41	0.45
1:D:13:HIS:O	1:D:17:MET:HG3	2.17	0.45
1:D:24:ILE:HG22	1:D:57:PHE:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:TYR:CZ	1:A:237:LEU:HD11	2.52	0.44
1:B:27:TYR:C	1:B:27:TYR:CD2	2.95	0.44
1:B:82:ASN:OD1	1:B:83:GLN:N	2.50	0.44
1:D:156:LEU:HD12	1:D:156:LEU:N	2.32	0.44
1:A:10:ILE:CG2	1:A:29:LEU:HD11	2.48	0.44
1:A:255:ARG:HH22	1:B:231:GLN:HE21	1.65	0.44
1:B:111:GLU:HG3	1:B:249:TYR:OH	2.18	0.44
1:D:127:VAL:O	1:D:153:CYS:HA	2.17	0.44
1:B:183:SER:O	1:B:184:THR:C	2.61	0.44
1:C:96:ARG:HD2	1:C:100:ASN:HD21	1.83	0.44
1:A:105:THR:O	1:A:109:ILE:HG13	2.17	0.44
1:B:32:GLU:OE2	1:B:32:GLU:N	2.30	0.44
1:D:128:TYR:CD1	1:D:154:GLU:HB2	2.52	0.44
1:D:224:HIS:CB	1:D:232:ARG:HG2	2.48	0.44
1:A:221:VAL:HG12	1:A:222:ALA:H	1.82	0.43
1:B:141:GLU:HA	1:B:144:LEU:HD13	2.00	0.43
1:B:215:TYR:N	1:B:215:TYR:CD1	2.84	0.43
1:D:236:GLN:HB3	1:D:240:LEU:HD23	2.00	0.43
1:D:70:ILE:HD12	1:D:70:ILE:HA	1.88	0.43
1:D:210:LYS:O	1:D:213:GLN:HG2	2.18	0.43
1:A:158:ASP:OD1	1:A:160:ASP:HB2	2.18	0.43
1:A:180:LEU:HD23	1:A:180:LEU:O	2.17	0.43
1:A:237:LEU:CD2	1:A:240:LEU:HD12	2.46	0.43
1:B:14:PHE:HD1	1:B:14:PHE:O	2.00	0.43
1:B:120:LEU:HD22	1:B:200:LYS:HE3	2.01	0.43
1:B:156:LEU:HD21	1:B:165:THR:CG2	2.42	0.43
1:A:71:PHE:CD1	1:A:71:PHE:C	2.95	0.43
1:A:127:VAL:HG13	1:A:153:CYS:HB3	1.99	0.43
1:B:93:ARG:NH1	1:B:231:GLN:OE1	2.51	0.43
1:D:175:VAL:HG12	1:D:201:THR:HG22	2.00	0.43
1:D:210:LYS:C	1:D:210:LYS:HD2	2.44	0.43
1:C:169:MET:HE1	1:C:194:ALA:HB2	1.99	0.43
1:B:82:ASN:OD1	1:B:82:ASN:C	2.62	0.43
1:B:146:PHE:HE2	1:B:247:TYR:HD2	1.66	0.43
1:B:156:LEU:CD2	1:B:165:THR:HG21	2.45	0.43
1:C:127:VAL:O	1:C:153:CYS:HA	2.18	0.43
1:D:101:MET:HG2	1:D:241:PHE:CE2	2.54	0.43
1:D:128:TYR:CE1	1:D:154:GLU:HB2	2.53	0.43
1:D:148:ARG:NH2	1:D:266:TRP:CH2	2.87	0.43
1:D:236:GLN:HB3	1:D:240:LEU:CD2	2.49	0.43
1:B:32:GLU:O	1:B:35:GLN:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:LEU:HD13	1:B:70:ILE:HD11	2.01	0.43
1:B:6:ILE:O	1:B:9:VAL:HG22	2.19	0.42
1:B:101:MET:CE	1:B:237:LEU:HB3	2.48	0.42
1:D:25:ALA:O	1:D:29:LEU:HG	2.18	0.42
1:D:54:LEU:HD21	1:D:66:TYR:CE1	2.54	0.42
1:A:138:VAL:CG2	1:A:236:GLN:HG2	2.42	0.42
1:B:15:GLU:C	1:B:17:MET:H	2.26	0.42
1:B:255:ARG:HD2	1:B:259:GLU:HG3	2.02	0.42
1:D:138:VAL:HG22	1:D:240:LEU:CD2	2.49	0.42
1:C:143:LYS:HE3	1:C:147:MET:HE1	2.01	0.42
1:C:102:ARG:NH2	1:C:103:GLU:HG2	2.34	0.42
1:B:147:MET:HE2	1:D:164:TRP:HB3	2.02	0.42
1:C:144:LEU:O	1:C:148:ARG:HG3	2.20	0.42
1:A:193:ASP:O	1:A:196:GLU:HG3	2.20	0.41
1:B:176:LEU:CD2	1:B:204:PHE:HE1	2.32	0.41
1:A:40:SER:HB2	1:A:51:GLN:OE1	2.20	0.41
1:B:128:TYR:CD1	1:B:169:MET:CE	3.03	0.41
1:D:5:ASP:OD1	1:D:7:ALA:N	2.53	0.41
1:D:110:ASP:OD1	1:D:112:VAL:HG22	2.20	0.41
1:B:249:TYR:CD1	1:B:249:TYR:N	2.87	0.41
1:C:224:HIS:CB	1:C:232:ARG:HD3	2.49	0.41
1:D:57:PHE:CD1	1:D:57:PHE:C	2.97	0.41
1:B:154:GLU:OE1	1:D:143:LYS:CE	2.67	0.41
1:C:137:LEU:CD2	1:D:137:LEU:O	2.68	0.41
1:D:130:PHE:CE1	1:D:156:LEU:HD13	2.55	0.41
1:A:233:ILE:HA	1:B:244:ASP:OD1	2.21	0.41
1:B:105:THR:OG1	1:B:242:PHE:CE1	2.73	0.41
1:B:202:VAL:HA	1:B:217:GLU:O	2.21	0.41
1:D:168:ILE:O	1:D:168:ILE:HG13	2.20	0.41
1:D:175:VAL:HG13	1:D:191:LEU:CD2	2.49	0.41
1:A:264:SER:HA	1:A:267:GLU:HB2	2.02	0.41
1:B:105:THR:O	1:B:109:ILE:HG13	2.21	0.41
1:B:80:GLN:O	1:B:81:ALA:HB3	2.21	0.41
1:A:47:LEU:HB2	1:A:49:ILE:HG23	2.02	0.41
1:B:102:ARG:O	1:B:105:THR:HG22	2.21	0.41
1:C:120:LEU:HD22	1:C:200:LYS:HZ3	1.86	0.41
1:C:171:GLU:HA	1:C:198:GLY:O	2.21	0.41
1:A:244:ASP:OD1	1:B:233:ILE:HA	2.21	0.41
1:D:28:PHE:CE2	1:D:69:PHE:HE2	2.39	0.41
1:A:221:VAL:HG12	1:A:222:ALA:N	2.35	0.40
1:A:265:TYR:CG	1:C:164:TRP:HZ3	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:TRP:HB3	1:D:147:MET:CE	2.51	0.40
1:C:96:ARG:HD2	1:C:100:ASN:ND2	2.37	0.40
1:C:128:TYR:HB3	1:C:130:PHE:HE1	1.87	0.40
1:C:185:PRO:O	1:C:186:SER:C	2.63	0.40
1:D:200:LYS:HD3	1:D:216:THR:HG21	2.04	0.40
1:A:212:SER:HB2	1:A:215:TYR:CE1	2.56	0.40
1:C:156:LEU:HD11	1:C:165:THR:CG2	2.41	0.40
1:A:41:GLN:O	1:A:45:GLN:HG2	2.20	0.40
1:C:155:ALA:C	1:C:156:LEU:HD23	2.46	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:THR:OG1	1:D:103:GLU:OE2[2_455]	2.09	0.11
1:A:18:THR:HG1	1:D:103:GLU:OE2[2_455]	1.58	0.02
1:D:66:TYR:N	2:A:303:PO4:O3[2_454]	2.19	0.01

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	264/283 (93%)	259 (98%)	5 (2%)	0	100	100
1	B	262/283 (93%)	250 (95%)	12 (5%)	0	100	100
1	C	182/283 (64%)	172 (94%)	10 (6%)	0	100	100
1	D	263/283 (93%)	257 (98%)	5 (2%)	1 (0%)	30	39
All	All	971/1132 (86%)	938 (97%)	32 (3%)	1 (0%)	48	61

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	40	SER

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	236/253 (93%)	232 (98%)	4 (2%)	53	72
1	B	233/253 (92%)	229 (98%)	4 (2%)	53	72
1	C	165/253 (65%)	160 (97%)	5 (3%)	36	53
1	D	236/253 (93%)	233 (99%)	3 (1%)	61	76
All	All	870/1012 (86%)	854 (98%)	16 (2%)	51	70

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

Mol	Chain	Res	Type
1	A	60	LYS
1	A	134	SER
1	A	181	SER
1	A	225	SER
1	B	74	GLN
1	B	183	SER
1	B	188	LEU
1	B	209	ASN
1	C	85	SER
1	C	169	MET
1	C	225	SER
1	C	237	LEU
1	C	258	LYS
1	D	78	GLU
1	D	233	ILE
1	D	237	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	ASN
1	A	113	GLN
1	B	100	ASN
1	B	224	HIS
1	B	236	GLN
1	C	87	HIS
1	C	119	GLN
1	D	30	GLN
1	D	42	GLN
1	D	80	GLN
1	D	82	ASN
1	D	83	GLN
1	D	213	GLN
1	D	263	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	PO4	A	301	-	4,4,4	0.88	0	6,6,6	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PO4	A	303	-	4,4,4	1.18	0	6,6,6	0.51	0
3	SO4	A	304	-	4,4,4	0.23	0	6,6,6	0.09	0
2	PO4	A	302	-	4,4,4	0.90	0	6,6,6	0.42	0
2	PO4	B	302	-	4,4,4	0.94	0	6,6,6	0.43	0
2	PO4	D	301	-	4,4,4	0.98	0	6,6,6	0.50	0
3	SO4	C	302	-	4,4,4	0.24	0	6,6,6	0.49	0
3	SO4	B	304	-	4,4,4	0.28	0	6,6,6	0.35	0
2	PO4	B	301	-	4,4,4	0.94	0	6,6,6	0.43	0
3	SO4	D	302	-	4,4,4	0.27	0	6,6,6	0.08	0
2	PO4	C	301	-	4,4,4	0.89	0	6,6,6	0.55	0
3	SO4	B	303	-	4,4,4	0.24	0	6,6,6	0.21	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	PO4	1	0
2	A	303	PO4	0	1
3	A	304	SO4	1	0
2	B	301	PO4	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	266/283 (93%)	0.62	11 (4%) 41 42	48, 78, 115, 166	0
1	B	264/283 (93%)	0.73	12 (4%) 38 38	51, 89, 139, 158	0
1	C	184/283 (65%)	0.45	7 (3%) 44 45	46, 72, 111, 132	0
1	D	265/283 (93%)	0.60	13 (4%) 35 34	44, 72, 113, 139	0
All	All	979/1132 (86%)	0.61	43 (4%) 39 39	44, 77, 126, 166	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	41	GLN	3.5
1	D	76	GLU	3.3
1	B	188	LEU	3.2
1	C	153	CYS	3.2
1	A	229	TYR	3.1
1	B	44	THR	3.1
1	A	47	LEU	3.0
1	C	220	LEU	2.9
1	B	162	PHE	2.8
1	A	237	LEU	2.8
1	B	237	LEU	2.7
1	B	12	SER	2.7
1	B	10	ILE	2.6
1	C	264	SER	2.6
1	D	83	GLN	2.6
1	A	2	ASP	2.5
1	A	160	ASP	2.5
1	B	81	ALA	2.5
1	B	249	TYR	2.4
1	D	4	PRO	2.4
1	D	45	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	164	TRP	2.4
1	D	6	ILE	2.3
1	D	47	LEU	2.3
1	B	82	ASN	2.3
1	C	203	LEU	2.3
1	B	79	ASN	2.3
1	D	39	SER	2.3
1	A	70	ILE	2.3
1	C	209	ASN	2.2
1	B	75	HIS	2.2
1	A	130	PHE	2.2
1	D	169	MET	2.2
1	D	164	TRP	2.2
1	C	249	TYR	2.1
1	A	48	HIS	2.1
1	A	10	ILE	2.1
1	A	81	ALA	2.1
1	B	130	PHE	2.0
1	D	249	TYR	2.0
1	C	219	VAL	2.0
1	D	43	VAL	2.0
1	D	257	SER	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 oligosaccharides 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	PO4	B	302	5/5	0.47	0.12	98,113,118,128	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	A	304	5/5	0.49	0.21	164,201,269,421	0
2	PO4	D	301	5/5	0.59	0.27	136,149,202,326	0
2	PO4	A	301	5/5	0.68	0.12	72,82,99,105	0
2	PO4	A	302	5/5	0.76	0.11	86,93,100,122	0
2	PO4	B	301	5/5	0.77	0.12	87,87,96,102	0
2	PO4	C	301	5/5	0.84	0.10	86,87,105,114	0
3	SO4	B	304	5/5	0.85	0.19	41,58,94,141	0
3	SO4	B	303	5/5	0.87	0.08	65,79,84,96	0
2	PO4	A	303	5/5	0.87	0.10	73,79,100,103	0
4	CL	D	303	1/1	0.87	0.11	58,58,58,58	0
4	CL	B	305	1/1	0.90	0.09	74,74,74,74	0
3	SO4	C	302	5/5	0.92	0.12	39,43,86,130	0
4	CL	A	305	1/1	0.92	0.08	67,67,67,67	0
3	SO4	D	302	5/5	0.93	0.06	71,71,83,85	0
4	CL	C	303	1/1	0.95	0.05	61,61,61,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.