



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:20 PM UTC

PDB ID : 3KU4 / pdb_00003ku4
Title : Trapping of an oxocarbenium ion intermediate in UP crystals
Authors : Paul, D.; O'Leary, S.; Rajashankar, K.; Bu, W.; Toms, A.; Settembre, E.;
Sanders, J.; Begley, T.P.; Ealick, S.E.
Deposited on : 2009-11-26
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

<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

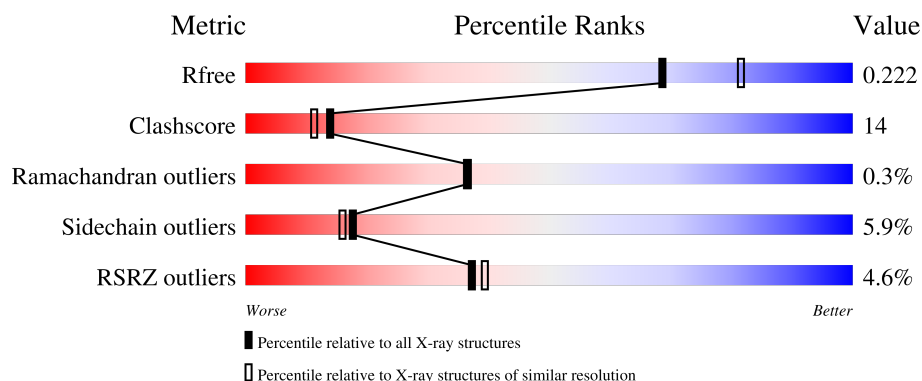
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 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	309	4% 69% 22% • 6%
1	B	309	6% 69% 22% • 5%
1	C	309	4% 69% 21% • 7%
1	D	309	4% 71% 19% • 7%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9822 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 Uridine phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	0	0	0
			2225	1408	381	414	22			
1	B	293	Total	C	N	O	S	0	0	0
			2242	1417	386	417	22			
1	C	287	Total	C	N	O	S	0	1	0
			2196	1392	373	408	23			
1	D	287	Total	C	N	O	S	0	0	0
			2185	1385	374	404	22			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

Continued on next page...

Continued from previous page...

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

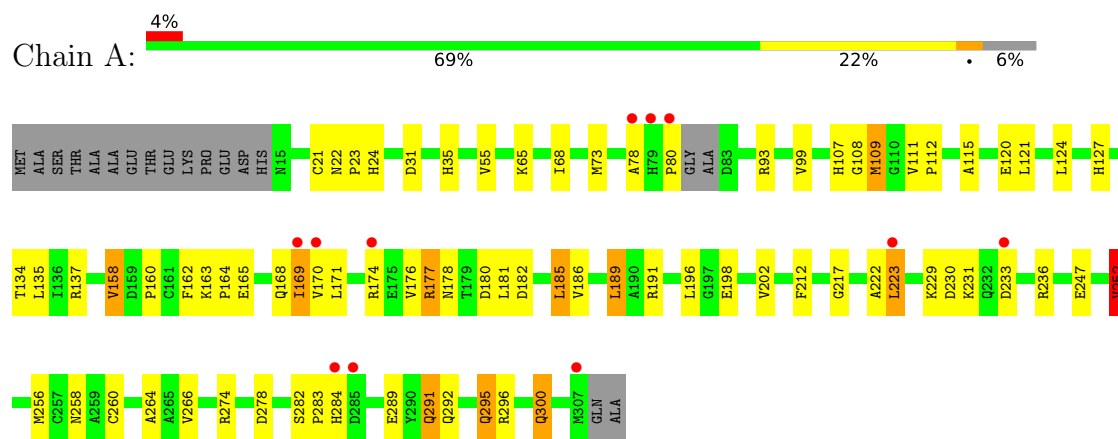
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	243	Total	O	0	0
			243	243		
3	B	264	Total	O	0	0
			264	264		
3	C	229	Total	O	0	0
			229	229		
3	D	218	Total	O	0	0
			218	218		

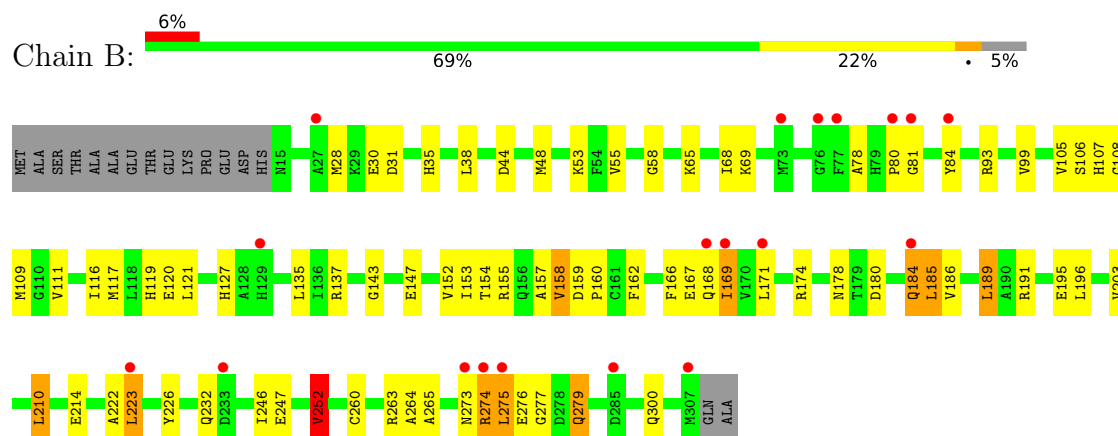
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

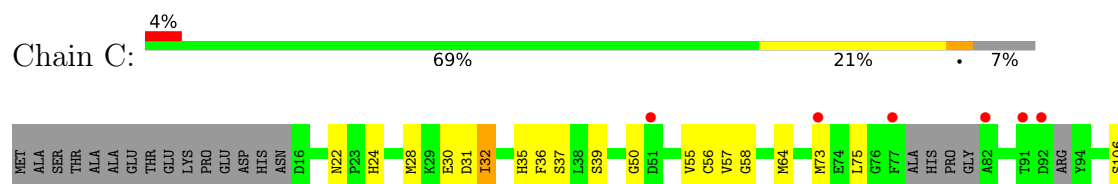
- Molecule 1: Uridine phosphorylase

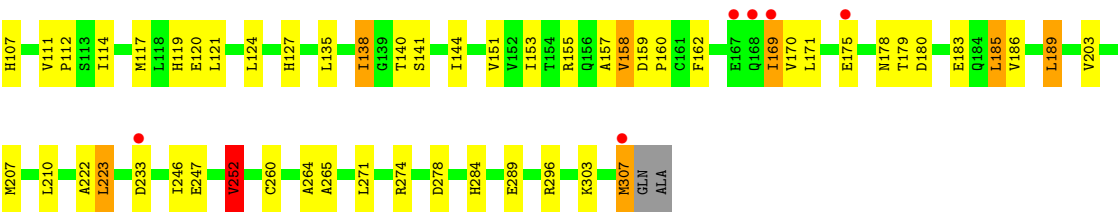


- Molecule 1: Uridine phosphorylase

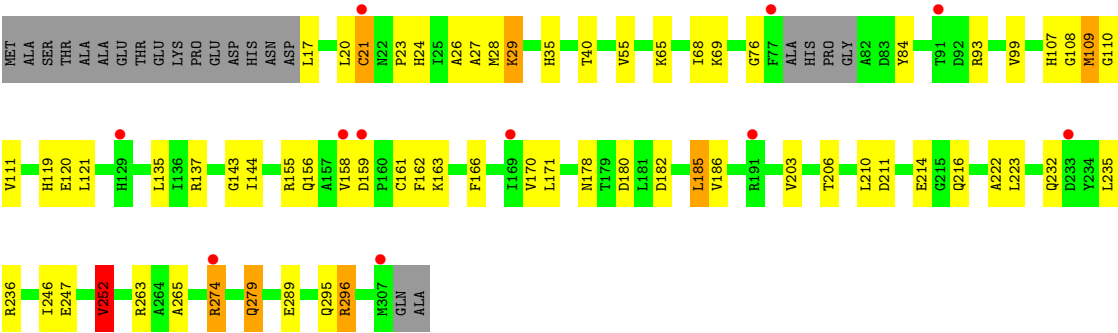


- Molecule 1: Uridine phosphorylase





● Molecule 1: Uridine phosphorylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	74.11Å 74.11Å 266.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 50.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.8 (50.00-2.10) 93.8 (50.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.02 (at 2.10Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.179 , 0.225 0.183 , 0.222	Depositor DCC
R_{free} test set	3904 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	22.9	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.048 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9822	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% 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: 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	0.66	1/2265 (0.0%)	0.82	2/3060 (0.1%)
1	B	0.80	8/2286 (0.3%)	0.87	7/3093 (0.2%)
1	C	0.67	1/2239 (0.0%)	0.84	6/3025 (0.2%)
1	D	0.49	0/2226	0.80	1/3010 (0.0%)
All	All	0.67	10/9016 (0.1%)	0.83	16/12188 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	169	ILE	CG1-CD1	21.24	2.34	1.51
1	C	169	ILE	CG1-CD1	20.57	2.31	1.51
1	B	169	ILE	CG1-CD1	20.16	2.30	1.51
1	B	155	ARG	C-O	-11.54	1.10	1.24
1	B	155	ARG	CZ-NH2	-10.38	1.20	1.33
1	B	155	ARG	CD-NE	-8.67	1.34	1.46
1	B	155	ARG	NE-CZ	-7.44	1.24	1.33
1	B	152	VAL	C-N	-5.95	1.25	1.33
1	B	155	ARG	N-CA	-5.60	1.39	1.46
1	B	154	THR	C-N	5.11	1.40	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	252	VAL	CB-CA-C	-7.98	101.36	112.14
1	C	169	ILE	CB-CG1-CD1	7.14	128.80	113.80
1	B	154	THR	CA-C-N	6.97	129.92	120.44
1	B	154	THR	C-N-CA	6.97	129.92	120.44
1	A	80	PRO	N-CA-CB	6.87	110.56	103.00
1	C	22	ASN	CA-C-N	6.57	126.27	119.56
1	C	22	ASN	C-N-CA	6.57	126.27	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	50	GLY	CA-C-N	6.27	129.31	120.28
1	C	50	GLY	C-N-CA	6.27	129.31	120.28
1	B	252	VAL	CB-CA-C	-6.10	102.70	112.16
1	B	154	THR	O-C-N	-6.08	114.56	122.77
1	B	157	ALA	N-CA-C	-6.01	101.59	110.48
1	D	252	VAL	CB-CA-C	-5.82	104.28	112.14
1	B	155	ARG	NE-CZ-NH2	-5.69	114.08	119.20
1	C	252	VAL	CB-CA-C	-5.11	105.24	112.14
1	B	105	VAL	N-CA-C	5.06	115.40	108.12

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	2225	0	2210	78	0
1	B	2242	0	2219	74	0
1	C	2196	0	2180	63	0
1	D	2185	0	2156	65	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	243	0	0	11	1
3	B	264	0	0	6	1
3	C	229	0	0	7	1
3	D	218	0	0	5	1
All	All	9822	0	8765	253	2

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 14.

All (253) 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:274:ARG:HG2	1:D:274:ARG:HH21	1.16	1.11
1:B:169:ILE:CG1	1:B:169:ILE:CD1	2.30	1.09
1:C:169:ILE:CD1	1:C:169:ILE:CG1	2.32	1.08
1:A:68:ILE:HD11	1:A:99:VAL:HG12	1.28	1.08
1:A:169:ILE:CD1	1:A:169:ILE:CG1	2.34	1.05
1:A:177:ARG:HG3	1:A:177:ARG:HH11	1.16	1.05
1:B:222:ALA:C	1:B:223:LEU:HD13	1.80	1.04
1:A:222:ALA:C	1:A:223:LEU:HD12	1.83	1.03
1:D:296:ARG:HH11	1:D:296:ARG:HB3	1.22	1.00
1:A:212:PHE:HB3	1:B:116:ILE:HD11	1.42	0.99
1:D:274:ARG:HG2	1:D:274:ARG:NH2	1.76	0.94
1:A:260:CYS:SG	1:B:223:LEU:HD11	2.08	0.93
1:A:68:ILE:CD1	1:A:99:VAL:HG12	1.99	0.91
1:D:274:ARG:HH21	1:D:274:ARG:CG	1.83	0.91
1:A:191:ARG:HB3	3:A:865:HOH:O	1.71	0.89
1:A:233:ASP:OD1	1:A:236:ARG:NH2	2.05	0.89
1:C:274:ARG:HD2	1:C:278:ASP:OD1	1.76	0.86
1:A:21:CYS:HB2	1:B:223:LEU:HD12	1.57	0.85
1:C:207:MET:HE2	1:C:246:ILE:HD12	1.59	0.84
1:C:119:HIS:HD2	1:D:222:ALA:H	1.27	0.82
1:C:107:HIS:HB3	1:C:117:MET:HE3	1.59	0.82
1:C:112:PRO:HB2	1:D:109:MET:HE1	1.60	0.81
1:B:222:ALA:O	1:B:223:LEU:HD13	1.81	0.81
1:A:160:PRO:HB2	1:B:169:ILE:HG21	1.62	0.81
1:B:107:HIS:HB3	1:B:117:MET:HE3	1.63	0.80
1:B:31:ASP:OD2	1:B:127:HIS:HE1	1.63	0.79
1:C:284:HIS:HD2	3:C:593:HOH:O	1.65	0.79
1:D:246:ILE:HD12	1:D:274:ARG:HE	1.48	0.78
1:D:296:ARG:HB3	1:D:296:ARG:NH1	1.99	0.77
1:B:274:ARG:O	1:B:277:GLY:N	2.17	0.77
1:C:185:LEU:HD13	1:C:265:ALA:HB2	1.67	0.76
1:A:35:HIS:HD2	1:A:120:GLU:OE2	1.69	0.76
1:A:177:ARG:HH11	1:A:177:ARG:CG	1.97	0.76
1:A:109:MET:HG2	1:B:93:ARG:CZ	2.17	0.75
1:C:56:CYS:SG	1:C:138:ILE:HD12	2.27	0.75
1:C:112:PRO:HB2	1:D:109:MET:CE	2.17	0.74
1:B:279:GLN:H	1:B:279:GLN:NE2	1.86	0.73
1:C:140:THR:HG23	1:C:271:LEU:HG	1.69	0.73
1:C:222:ALA:H	1:D:119:HIS:HD2	1.36	0.73
1:A:111:VAL:HG22	1:A:252:VAL:HG22	1.71	0.72
1:A:222:ALA:H	1:B:119:HIS:HD2	1.36	0.72
1:C:31:ASP:OD2	1:C:127:HIS:HE1	1.71	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:HIS:HD2	1:C:120:GLU:OE2	1.71	0.72
3:C:321:HOH:O	1:D:119:HIS:HE1	1.72	0.71
1:C:274:ARG:HD3	3:C:918:HOH:O	1.89	0.71
1:D:24:HIS:O	1:D:28:MET:HG3	1.91	0.71
1:D:111:VAL:HG22	1:D:252:VAL:HG22	1.71	0.71
1:C:170:VAL:O	1:C:171:LEU:HB2	1.89	0.71
1:A:115:ALA:HB1	1:A:256:MET:HE1	1.73	0.71
1:D:35:HIS:HD2	1:D:120:GLU:OE2	1.74	0.71
1:A:170:VAL:O	1:A:171:LEU:HB2	1.89	0.71
1:A:229:LYS:O	1:A:229:LYS:HD3	1.92	0.70
1:A:112:PRO:HG3	1:B:210:LEU:HD22	1.72	0.70
1:A:212:PHE:CB	1:B:116:ILE:HD11	2.19	0.70
1:B:246:ILE:HD12	1:B:274:ARG:CD	2.22	0.70
1:D:29:LYS:HB2	1:D:29:LYS:NZ	2.06	0.70
1:C:138:ILE:HD13	1:C:138:ILE:H	1.56	0.70
1:A:178:ASN:ND2	1:A:180:ASP:H	1.88	0.69
1:C:178:ASN:HD21	1:C:180:ASP:HB2	1.58	0.69
1:D:232:GLN:O	1:D:236:ARG:HG2	1.93	0.69
1:A:177:ARG:HG3	1:A:177:ARG:NH1	1.96	0.68
1:A:223:LEU:HD12	1:A:223:LEU:N	2.08	0.68
1:D:216:GLN:O	1:D:274:ARG:NH1	2.27	0.68
1:D:216:GLN:HB3	1:D:274:ARG:NH1	2.08	0.67
1:A:256:MET:HE3	3:A:952:HOH:O	1.94	0.67
1:A:185:LEU:HD22	1:A:189:LEU:HD22	1.76	0.67
1:D:161:CYS:HB2	1:D:163:LYS:HD3	1.77	0.67
1:C:233:ASP:OD1	3:C:316:HOH:O	2.13	0.66
1:A:169:ILE:HD12	3:A:388:HOH:O	1.96	0.66
1:A:55:VAL:HG11	1:A:121:LEU:HD21	1.78	0.66
1:C:260:CYS:SG	1:D:223:LEU:HD21	2.36	0.65
1:B:273:ASN:O	1:B:275:LEU:N	2.30	0.65
1:C:119:HIS:CD2	1:D:222:ALA:H	2.14	0.65
1:B:55:VAL:HG13	3:B:402:HOH:O	1.97	0.65
1:B:274:ARG:O	1:B:275:LEU:C	2.39	0.64
1:B:147:GLU:HG2	3:B:339:HOH:O	1.97	0.64
1:B:167:GLU:OE1	1:B:174:ARG:HD3	2.00	0.62
1:D:159:ASP:HB3	1:D:161:CYS:H	1.63	0.62
1:B:44:ASP:O	1:B:48:MET:HG3	2.00	0.61
1:C:57:VAL:O	1:C:138:ILE:HD13	2.00	0.61
1:C:222:ALA:C	1:C:223:LEU:HD12	2.26	0.61
1:D:107:HIS:HE1	1:D:137:ARG:HH11	1.49	0.61
1:B:107:HIS:HB3	1:B:117:MET:CE	2.31	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:HIS:HD2	1:D:222:ALA:N	1.98	0.60
1:B:273:ASN:O	1:B:274:ARG:C	2.43	0.60
1:C:55:VAL:HG11	1:C:121:LEU:HD21	1.82	0.60
1:A:223:LEU:N	1:A:223:LEU:CD1	2.63	0.60
1:B:158:VAL:HG13	1:B:162:PHE:HA	1.84	0.60
1:A:107:HIS:HD2	1:A:108:GLY:O	1.85	0.60
1:C:64:MET:HE1	1:C:138:ILE:HD11	1.84	0.60
1:C:24:HIS:O	1:C:28:MET:HG3	2.02	0.59
1:A:31:ASP:OD2	1:A:127:HIS:HE1	1.85	0.59
1:D:107:HIS:HD2	1:D:108:GLY:O	1.85	0.59
1:D:111:VAL:HG22	1:D:252:VAL:CG2	2.33	0.59
1:B:223:LEU:HD13	1:B:223:LEU:N	2.14	0.59
1:B:275:LEU:C	1:B:277:GLY:H	2.11	0.59
1:B:78:ALA:HB3	3:B:754:HOH:O	2.03	0.59
1:C:127:HIS:HD2	3:C:503:HOH:O	1.84	0.59
1:A:169:ILE:CD1	3:A:388:HOH:O	2.50	0.58
3:A:314:HOH:O	1:B:119:HIS:HE1	1.87	0.58
1:B:28:MET:HE2	1:B:30:GLU:O	2.03	0.58
1:B:185:LEU:HD13	1:B:265:ALA:HB2	1.86	0.58
1:B:55:VAL:HG11	1:B:121:LEU:HD21	1.85	0.58
1:D:185:LEU:HD13	1:D:265:ALA:HB2	1.86	0.57
1:C:107:HIS:CG	1:C:114:ILE:HD13	2.39	0.57
1:D:296:ARG:HH11	1:D:296:ARG:CB	2.08	0.57
1:A:256:MET:CE	3:A:952:HOH:O	2.50	0.56
1:A:284:HIS:HB2	3:A:350:HOH:O	2.05	0.56
1:C:111:VAL:HG22	1:C:252:VAL:CG2	2.35	0.56
1:C:140:THR:CG2	1:C:141:SER:N	2.69	0.56
1:B:274:ARG:O	1:B:277:GLY:O	2.24	0.56
1:D:143:GLY:O	1:D:144:ILE:HD13	2.05	0.55
1:C:111:VAL:HG13	1:C:252:VAL:HG21	1.88	0.55
1:B:246:ILE:HD12	1:B:274:ARG:NE	2.22	0.55
1:C:140:THR:HG22	1:C:141:SER:N	2.22	0.55
1:B:166:PHE:CZ	1:B:252:VAL:HG13	2.42	0.54
1:D:166:PHE:CZ	1:D:252:VAL:HG13	2.42	0.54
1:A:134:THR:HG23	1:A:185:LEU:HD11	1.88	0.54
1:A:274:ARG:NH2	1:A:278:ASP:OD1	2.40	0.54
1:B:107:HIS:HD2	1:B:108:GLY:O	1.91	0.54
1:A:191:ARG:HD2	3:A:865:HOH:O	2.07	0.54
1:A:65:LYS:O	1:A:68:ILE:HG22	2.08	0.54
1:A:222:ALA:O	1:A:223:LEU:HD12	2.07	0.54
1:D:76:GLY:HA2	3:D:665:HOH:O	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:HIS:HD2	1:B:120:GLU:OE2	1.91	0.53
1:B:107:HIS:HE1	1:B:137:ARG:HH11	1.57	0.53
1:C:112:PRO:CB	1:D:109:MET:HE1	2.35	0.53
1:D:279:GLN:H	1:D:279:GLN:NE2	2.06	0.53
1:D:55:VAL:HG11	1:D:121:LEU:HD21	1.90	0.52
1:D:166:PHE:HD1	3:D:354:HOH:O	1.92	0.52
1:A:196:LEU:HD21	1:A:300:GLN:HG3	1.91	0.52
1:B:153:ILE:HD13	1:B:189:LEU:HB3	1.91	0.52
1:B:222:ALA:O	1:B:223:LEU:CD1	2.53	0.52
1:D:17:LEU:N	3:D:735:HOH:O	2.42	0.52
1:B:178:ASN:ND2	1:B:180:ASP:H	2.07	0.51
1:A:295:GLN:NE2	3:A:490:HOH:O	2.43	0.51
1:D:158:VAL:HG22	1:D:206:THR:O	2.10	0.51
1:C:107:HIS:CB	1:C:114:ILE:HD13	2.40	0.51
1:A:222:ALA:H	1:B:119:HIS:CD2	2.24	0.51
1:C:58:GLY:O	1:C:106:SER:HA	2.11	0.51
1:C:140:THR:CG2	1:C:271:LEU:HG	2.38	0.50
1:A:181:LEU:HD21	1:A:266:VAL:HG23	1.93	0.50
1:A:222:ALA:N	1:B:119:HIS:HD2	2.05	0.50
1:D:279:GLN:H	1:D:279:GLN:CD	2.20	0.50
1:A:158:VAL:CG1	1:A:162:PHE:HA	2.42	0.50
1:B:275:LEU:O	1:B:277:GLY:N	2.45	0.49
1:A:222:ALA:C	1:A:223:LEU:CD1	2.71	0.49
1:A:168:GLN:NE2	1:B:214:GLU:OE2	2.44	0.49
1:C:111:VAL:HB	1:C:112:PRO:HD3	1.93	0.49
1:D:246:ILE:CD1	1:D:274:ARG:HE	2.21	0.49
1:D:144:ILE:HD13	1:D:274:ARG:HB2	1.94	0.49
1:C:303:LYS:O	1:C:307:MET:SD	2.71	0.49
1:A:177:ARG:CG	1:A:177:ARG:NH1	2.65	0.49
1:C:223:LEU:HD12	1:C:223:LEU:N	2.27	0.49
1:A:111:VAL:HG22	1:A:252:VAL:CG2	2.40	0.48
1:B:65:LYS:HE2	1:B:69:LYS:HE3	1.95	0.48
1:B:184:GLN:CG	1:B:263:ARG:HH22	2.26	0.48
1:B:159:ASP:HB2	1:B:160:PRO:CD	2.44	0.48
1:D:178:ASN:ND2	1:D:180:ASP:H	2.12	0.48
1:A:170:VAL:O	1:A:171:LEU:CB	2.59	0.48
1:D:274:ARG:NH2	1:D:274:ARG:CG	2.50	0.48
1:D:211:ASP:OD2	1:D:214:GLU:HB2	2.13	0.48
1:C:107:HIS:HB3	1:C:117:MET:CE	2.37	0.47
1:C:274:ARG:CD	1:C:278:ASP:OD1	2.55	0.47
1:D:26:ALA:HB3	3:D:459:HOH:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:ALA:N	1:D:119:HIS:HD2	2.09	0.47
1:A:178:ASN:HD21	1:A:180:ASP:CB	2.27	0.47
1:D:235:LEU:HD13	1:D:274:ARG:HB3	1.96	0.47
1:B:275:LEU:C	1:B:277:GLY:N	2.70	0.47
1:C:207:MET:HB3	1:C:246:ILE:CD1	2.45	0.47
1:C:32:ILE:HD13	1:C:39:SER:HB2	1.96	0.47
1:A:217:GLY:O	1:A:231:LYS:HD3	2.14	0.47
1:A:107:HIS:HE1	1:A:137:ARG:HH11	1.63	0.47
1:A:124:LEU:C	1:A:124:LEU:HD23	2.40	0.46
1:B:111:VAL:HG22	1:B:252:VAL:HG22	1.96	0.46
1:D:21:CYS:O	1:D:23:PRO:HD3	2.15	0.46
1:C:73:MET:HG2	3:C:443:HOH:O	2.15	0.46
1:C:151:VAL:HG21	3:C:749:HOH:O	2.14	0.46
1:A:24:HIS:HE1	1:B:226:TYR:O	1.98	0.46
1:D:29:LYS:HB2	1:D:29:LYS:HZ3	1.79	0.46
1:D:69:LYS:HG2	1:D:84:TYR:CE2	2.50	0.46
1:D:107:HIS:CE1	1:D:137:ARG:HH11	2.32	0.46
1:A:158:VAL:HG13	1:A:162:PHE:HA	1.98	0.46
1:D:109:MET:HE3	1:D:109:MET:C	2.39	0.46
1:C:144:ILE:HD11	1:C:246:ILE:HD11	1.98	0.46
1:B:53:LYS:HD2	3:B:326:HOH:O	2.16	0.46
1:B:158:VAL:CG1	1:B:162:PHE:HA	2.45	0.46
1:B:232:GLN:NE2	1:B:275:LEU:O	2.49	0.45
1:A:178:ASN:HD21	1:A:180:ASP:CG	2.25	0.45
1:D:29:LYS:HB2	1:D:29:LYS:HZ2	1.78	0.45
1:A:178:ASN:HD21	1:A:180:ASP:H	1.60	0.45
1:A:182:ASP:OD1	1:A:185:LEU:HB2	2.16	0.45
1:C:36:PHE:O	1:C:37:SER:HB2	2.16	0.45
1:B:279:GLN:H	1:B:279:GLN:HE21	1.61	0.45
1:C:124:LEU:HD23	1:C:124:LEU:C	2.42	0.45
1:A:135:LEU:O	1:A:264:ALA:HA	2.18	0.44
1:B:48:MET:HE3	1:D:27:ALA:HB2	1.99	0.44
1:D:68:ILE:HD11	1:D:99:VAL:HG12	1.98	0.44
1:A:292:GLN:HG3	3:A:352:HOH:O	2.16	0.44
1:C:140:THR:HG21	1:C:271:LEU:CD1	2.47	0.44
1:C:210:LEU:CD2	1:D:210:LEU:HD11	2.48	0.44
1:C:178:ASN:ND2	1:C:180:ASP:H	2.16	0.44
1:A:163:LYS:HA	1:A:164:PRO:HD3	1.83	0.44
1:C:159:ASP:HB2	1:C:160:PRO:CD	2.48	0.44
1:B:68:ILE:HD11	1:B:99:VAL:HG12	1.99	0.43
1:B:273:ASN:O	1:B:273:ASN:OD1	2.36	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:MET:HA	1:A:78:ALA:HB2	2.00	0.43
1:C:30:GLU:OE2	1:C:32:ILE:HD11	2.19	0.43
1:A:284:HIS:CD2	3:A:739:HOH:O	2.71	0.43
1:A:291:GLN:HE21	1:A:291:GLN:HB2	1.47	0.43
1:B:196:LEU:HD21	1:B:300:GLN:HG3	2.00	0.43
1:D:93:ARG:HD2	3:D:700:HOH:O	2.18	0.43
1:D:156:GLN:HG2	1:D:180:ASP:OD1	2.19	0.43
1:C:157:ALA:HB3	1:C:179:THR:HB	2.01	0.43
1:B:84:TYR:CD2	1:B:84:TYR:N	2.86	0.42
1:B:246:ILE:HD12	1:B:274:ARG:HD2	1.99	0.42
1:A:282:SER:HA	1:A:283:PRO:HD3	1.83	0.42
1:B:143:GLY:O	1:B:274:ARG:HG3	2.19	0.42
1:C:55:VAL:HB	1:C:135:LEU:HG	1.99	0.42
1:D:162:PHE:N	1:D:162:PHE:CD2	2.84	0.42
1:D:170:VAL:O	1:D:171:LEU:HB2	2.18	0.42
1:B:80:PRO:HA	1:B:81:GLY:HA2	1.71	0.42
1:B:159:ASP:HB2	1:B:160:PRO:HD2	2.01	0.42
1:C:153:ILE:HD13	1:C:189:LEU:HB3	2.02	0.42
1:D:159:ASP:HB2	1:D:163:LYS:H	1.83	0.42
1:A:165:GLU:HB3	1:A:176:VAL:HG13	2.02	0.42
1:A:198:GLU:OE1	1:A:296:ARG:NH1	2.53	0.42
1:A:22:ASN:HA	1:A:23:PRO:HD2	1.91	0.42
1:A:212:PHE:CD1	1:B:116:ILE:HD11	2.55	0.42
1:C:289:GLU:OE1	1:C:296:ARG:NH2	2.48	0.42
1:B:55:VAL:CG1	3:B:402:HOH:O	2.59	0.42
1:C:135:LEU:O	1:C:264:ALA:HA	2.20	0.42
1:A:93:ARG:CZ	1:B:109:MET:HE3	2.50	0.42
1:A:258:ASN:HD22	1:A:258:ASN:HA	1.60	0.42
1:A:230:ASP:HB3	1:B:171:LEU:HD11	2.02	0.41
1:B:35:HIS:HE1	3:B:898:HOH:O	2.02	0.41
1:A:158:VAL:HG22	1:A:163:LYS:C	2.45	0.41
1:B:58:GLY:O	1:B:106:SER:HA	2.21	0.41
1:C:75:LEU:HD23	1:C:75:LEU:HA	1.88	0.41
1:D:65:LYS:O	1:D:68:ILE:HG22	2.20	0.41
1:A:181:LEU:CD2	1:A:266:VAL:HG23	2.50	0.41
1:A:229:LYS:HD3	1:A:229:LYS:C	2.43	0.41
1:C:158:VAL:HG13	1:C:162:PHE:HA	2.03	0.41
1:A:223:LEU:HD11	1:B:260:CYS:SG	2.61	0.41
1:D:55:VAL:HB	1:D:135:LEU:HG	2.03	0.41
1:A:162:PHE:CD2	1:A:162:PHE:N	2.86	0.41
1:D:246:ILE:HD12	1:D:274:ARG:NE	2.27	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:VAL:O	1:B:99:VAL:HG13	2.22	0.40
1:D:182:ASP:OD2	1:D:263:ARG:HD2	2.21	0.40
1:B:135:LEU:O	1:B:264:ALA:HA	2.21	0.40
1:C:155:ARG:NH1	1:C:183:GLU:OE2	2.54	0.40
1:D:109:MET:HE3	1:D:110:GLY:HA3	2.04	0.40
1:B:191:ARG:O	1:B:195:GLU:HG3	2.22	0.40

All (2) 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)
3:C:358:HOH:O	3:D:357:HOH:O[4_564]	2.09	0.11
3:A:376:HOH:O	3:B:375:HOH:O[4_554]	2.13	0.07

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	287/309 (93%)	283 (99%)	4 (1%)	0	100	100
1	B	291/309 (94%)	282 (97%)	6 (2%)	3 (1%)	12	9
1	C	282/309 (91%)	275 (98%)	7 (2%)	0	100	100
1	D	283/309 (92%)	281 (99%)	2 (1%)	0	100	100
All	All	1143/1236 (92%)	1121 (98%)	19 (2%)	3 (0%)	36	36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	274	ARG
1	B	275	LEU
1	B	276	GLU

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	239/255 (94%)	224 (94%)	15 (6%)	16	14
1	B	241/255 (94%)	228 (95%)	13 (5%)	20	18
1	C	237/255 (93%)	225 (95%)	12 (5%)	21	21
1	D	232/255 (91%)	216 (93%)	16 (7%)	14	12
All	All	949/1020 (93%)	893 (94%)	56 (6%)	18	16

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	MET
1	A	158	VAL
1	A	174	ARG
1	A	177	ARG
1	A	185	LEU
1	A	186	VAL
1	A	189	LEU
1	A	202	VAL
1	A	223	LEU
1	A	247	GLU
1	A	252	VAL
1	A	289	GLU
1	A	291	GLN
1	A	295	GLN
1	A	300	GLN
1	B	38	LEU
1	B	158	VAL
1	B	168	GLN
1	B	184	GLN
1	B	185	LEU
1	B	186	VAL
1	B	189	LEU
1	B	203	VAL
1	B	210	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	223	LEU
1	B	247	GLU
1	B	252	VAL
1	B	279	GLN
1	C	32	ILE
1	C	138	ILE
1	C	158	VAL
1	C	175	GLU
1	C	185	LEU
1	C	186	VAL
1	C	189	LEU
1	C	203	VAL
1	C	223	LEU
1	C	247	GLU
1	C	252	VAL
1	C	307	MET
1	D	20	LEU
1	D	21	CYS
1	D	29	LYS
1	D	40	THR
1	D	109	MET
1	D	155	ARG
1	D	185	LEU
1	D	186	VAL
1	D	203	VAL
1	D	247	GLU
1	D	252	VAL
1	D	274	ARG
1	D	279	GLN
1	D	289	GLU
1	D	295	GLN
1	D	296	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	HIS
1	A	35	HIS
1	A	107	HIS
1	A	127	HIS
1	A	178	ASN
1	A	258	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	291	GLN
1	A	295	GLN
1	B	15	ASN
1	B	35	HIS
1	B	79	HIS
1	B	107	HIS
1	B	119	HIS
1	B	127	HIS
1	B	168	GLN
1	B	178	ASN
1	B	184	GLN
1	B	279	GLN
1	C	35	HIS
1	C	119	HIS
1	C	127	HIS
1	C	168	GLN
1	C	178	ASN
1	C	284	HIS
1	D	35	HIS
1	D	107	HIS
1	D	119	HIS
1	D	178	ASN
1	D	187	GLN
1	D	279	GLN
1	D	295	GLN
1	D	300	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	C	310	-	4,4,4	0.29	0	6,6,6	0.24	0
2	SO4	B	310	-	4,4,4	0.28	0	6,6,6	0.21	0
2	SO4	D	310	-	4,4,4	0.19	0	6,6,6	0.50	0
2	SO4	A	310	-	4,4,4	0.37	0	6,6,6	0.19	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.

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

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	291/309 (94%)	0.07	11 (3%)	44 46	15, 23, 41, 64	0
1	B	293/309 (94%)	0.03	19 (6%)	25 26	14, 21, 38, 54	0
1	C	287/309 (92%)	-0.01	12 (4%)	40 42	14, 21, 39, 56	1 (0%)
1	D	287/309 (92%)	0.02	11 (3%)	44 46	14, 23, 39, 51	0
All	All	1158/1236 (93%)	0.03	53 (4%)	37 39	14, 22, 39, 64	1 (0%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	274	ARG	8.0
1	B	275	LEU	5.5
1	A	285	ASP	5.1
1	D	21	CYS	4.8
1	A	233	ASP	4.4
1	D	169	ILE	4.2
1	C	307	MET	4.0
1	A	78	ALA	3.8
1	A	284	HIS	3.7
1	B	233	ASP	3.7
1	B	81	GLY	3.7
1	A	79	HIS	3.6
1	D	159	ASP	3.5
1	D	233	ASP	3.4
1	B	223	LEU	3.3
1	A	307	MET	3.3
1	B	307	MET	3.2
1	A	80	PRO	3.0
1	B	273	ASN	3.0
1	D	274	ARG	2.9
1	C	51	ASP	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	171	LEU	2.8
1	B	80	PRO	2.8
1	C	233	ASP	2.7
1	C	91	THR	2.7
1	D	158	VAL	2.7
1	D	191	ARG	2.7
1	B	168	GLN	2.6
1	B	27	ALA	2.6
1	D	91	THR	2.6
1	A	223	LEU	2.6
1	B	285	ASP	2.5
1	B	77	PHE	2.5
1	A	169	ILE	2.5
1	D	307	MET	2.5
1	B	184	GLN	2.4
1	D	77	PHE	2.4
1	C	82	ALA	2.3
1	B	73	MET	2.3
1	B	76	GLY	2.3
1	C	92	ASP	2.2
1	C	169	ILE	2.2
1	A	170	VAL	2.2
1	C	175	GLU	2.2
1	A	174	ARG	2.2
1	C	73	MET	2.1
1	B	169	ILE	2.1
1	C	167	GLU	2.1
1	D	129	HIS	2.1
1	C	77	PHE	2.0
1	C	168	GLN	2.0
1	B	129	HIS	2.0
1	B	84	TYR	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($\text{\AA}^2$)	Q<0.9
2	SO4	A	310	5/5	0.85	0.16	31,37,48,52	0
2	SO4	D	310	5/5	0.96	0.09	25,26,31,31	0
2	SO4	B	310	5/5	0.98	0.06	18,22,24,26	0
2	SO4	C	310	5/5	0.99	0.08	25,26,30,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.