



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 09:37 AM UTC

PDB ID : 9IZ3 / pdb_00009iz3
Title : Crystal structure of phosphonopyruvate decarboxylase RhiEF from *Bacillus subtilis* ATCC6633
Authors : Nakamura, A.; Kojima, S.
Deposited on : 2024-07-31
Resolution : 2.46 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

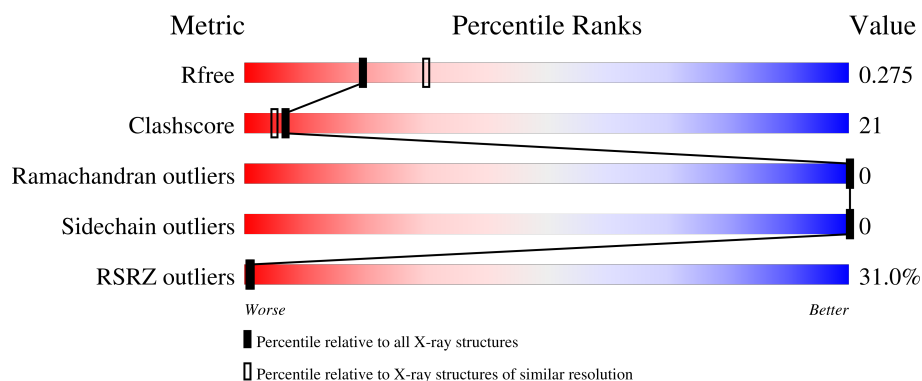
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.46 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	181	33% 45% 33% 22%
1	C	181	38% 39% 40% 20%
2	B	186	9% 72% 22% 6%
2	D	186	27% 59% 33% 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4984 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 Putative phosphonopyruvate decarboxylase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	142	Total	C	N	O	S	0	0	0
			1110	715	176	212	7			
1	C	144	Total	C	N	O	S	0	0	0
			1135	732	182	214	7			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP D4HRI2
A	-12	GLY	-	expression tag	UNP D4HRI2
A	-11	SER	-	expression tag	UNP D4HRI2
A	-10	SER	-	expression tag	UNP D4HRI2
A	-9	HIS	-	expression tag	UNP D4HRI2
A	-8	HIS	-	expression tag	UNP D4HRI2
A	-7	HIS	-	expression tag	UNP D4HRI2
A	-6	HIS	-	expression tag	UNP D4HRI2
A	-5	HIS	-	expression tag	UNP D4HRI2
A	-4	HIS	-	expression tag	UNP D4HRI2
A	-3	SER	-	expression tag	UNP D4HRI2
A	-2	GLN	-	expression tag	UNP D4HRI2
A	-1	ASP	-	expression tag	UNP D4HRI2
A	0	PRO	-	expression tag	UNP D4HRI2
C	-13	MET	-	initiating methionine	UNP D4HRI2
C	-12	GLY	-	expression tag	UNP D4HRI2
C	-11	SER	-	expression tag	UNP D4HRI2
C	-10	SER	-	expression tag	UNP D4HRI2
C	-9	HIS	-	expression tag	UNP D4HRI2
C	-8	HIS	-	expression tag	UNP D4HRI2
C	-7	HIS	-	expression tag	UNP D4HRI2
C	-6	HIS	-	expression tag	UNP D4HRI2
C	-5	HIS	-	expression tag	UNP D4HRI2
C	-4	HIS	-	expression tag	UNP D4HRI2
C	-3	SER	-	expression tag	UNP D4HRI2

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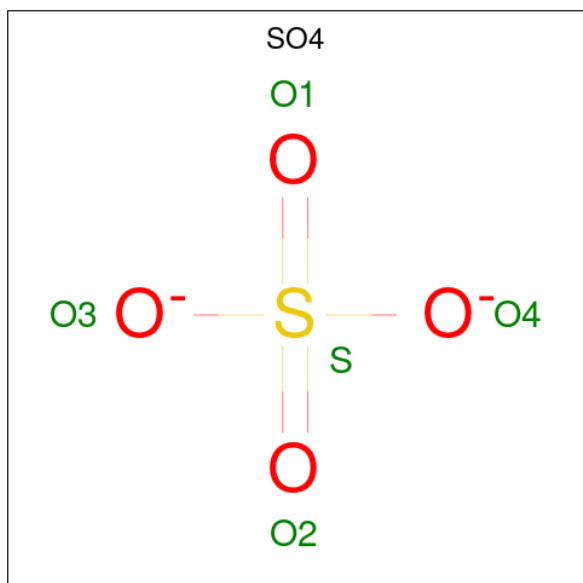
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLN	-	expression tag	UNP D4HRI2
C	-1	ASP	-	expression tag	UNP D4HRI2
C	0	PRO	-	expression tag	UNP D4HRI2

- Molecule 2 is a protein called Putative phosphonopyruvate decarboxylase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	174	Total	C	N	O	S	0	0	0
			1356	865	233	249	9			
2	D	172	Total	C	N	O	S	0	0	0
			1338	854	228	247	9			

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



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

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

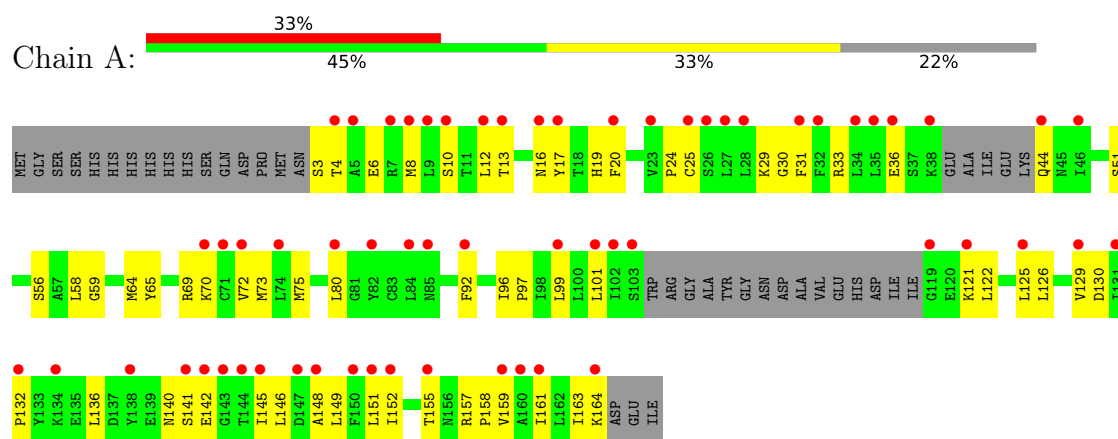
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	9	Total	O	0	0
			9	9		
4	D	1	Total	O	0	0
			1	1		

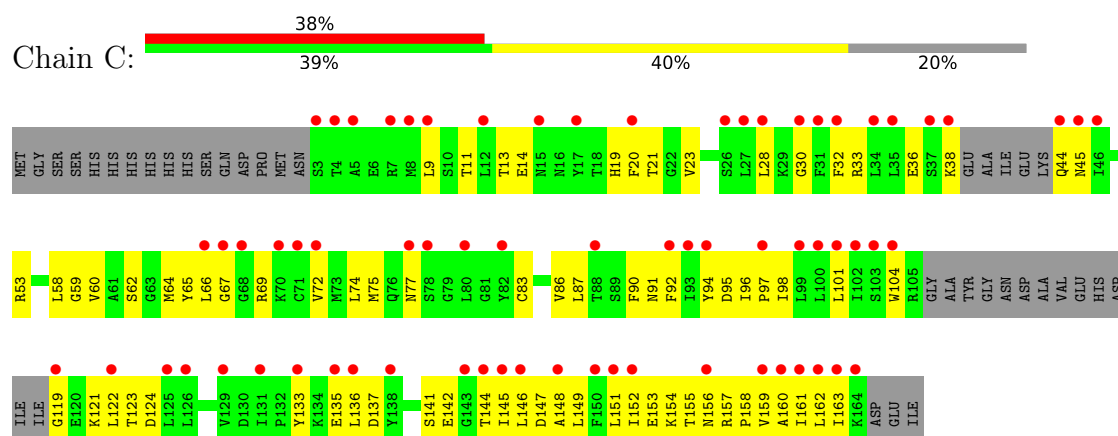
3 Residue-property plots [i](#)

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.

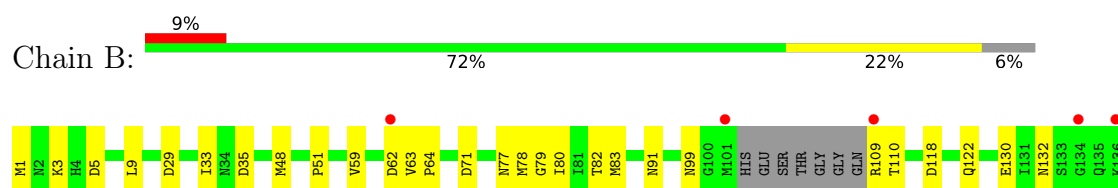
- Molecule 1: Putative phosphonopyruvate decarboxylase alpha subunit

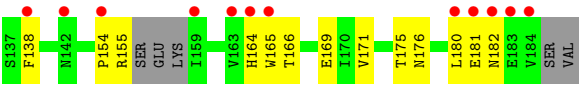


- Molecule 1: Putative phosphonopyruvate decarboxylase alpha subunit

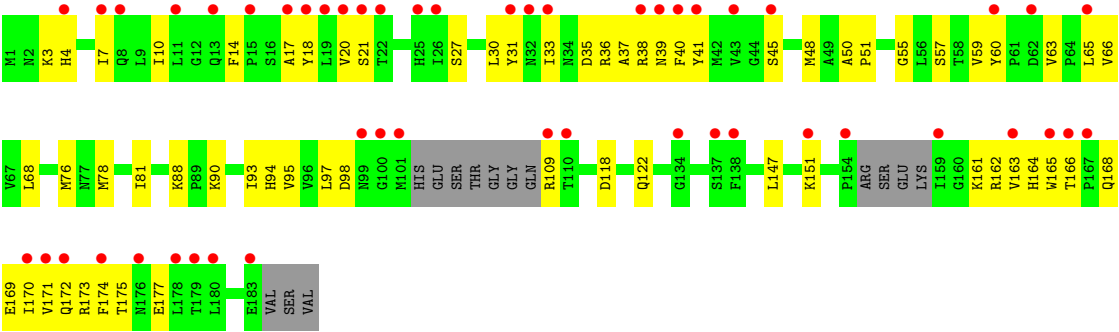


- Molecule 2: Putative phosphonopyruvate decarboxylase beta subunit





● Molecule 2: Putative phosphonopyruvate decarboxylase beta subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	176.99Å 176.99Å 68.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.98 – 2.46 40.98 – 2.46	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.98-2.46) 99.7 (40.98-2.46)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.239 , 0.272 0.242 , 0.275	Depositor DCC
R_{free} test set	2225 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	59.6	Xtriage
Anisotropy	0.446	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 91.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4984	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% 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: 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	0.30	1/1126 (0.1%)	0.51	0/1520
1	C	0.29	0/1153	0.59	0/1557
2	B	0.19	0/1383	0.40	0/1875
2	D	0.27	0/1365	0.51	0/1851
All	All	0.26	1/5027 (0.0%)	0.50	0/6803

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	140	ASN	CA-CB	6.67	1.64	1.53

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	1110	0	1133	56	0
1	C	1135	0	1156	69	0
2	B	1356	0	1361	31	0
2	D	1338	0	1339	71	0
3	B	20	0	0	0	0
3	D	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	9	0	0	1	0
4	D	1	0	0	0	0
All	All	4984	0	4989	213	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 21.

All (213) 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)
2:D:18:TYR:HD1	2:D:38:ARG:HB2	1.31	0.94
1:A:24:PRO:HB3	2:D:109:ARG:HH22	1.34	0.92
1:C:144:THR:HA	1:C:147:ASP:HB2	1.55	0.89
1:A:72:VAL:HG22	1:A:99:LEU:HB3	1.54	0.89
1:C:121:LYS:H	1:C:121:LYS:HD3	1.38	0.88
1:C:11:THR:HG21	1:C:142:GLU:HG3	1.56	0.87
1:C:20:PHE:CD1	1:C:72:VAL:HG22	2.11	0.86
2:D:10:ILE:HD12	2:D:95:VAL:HG21	1.59	0.84
2:D:18:TYR:CD1	2:D:38:ARG:HB2	2.15	0.81
2:D:7:ILE:HA	2:D:10:ILE:HG22	1.63	0.80
2:D:31:TYR:CD1	2:D:35:ASP:HB2	2.18	0.79
1:A:142:GLU:HA	1:A:145:ILE:HG12	1.64	0.78
2:D:166:THR:HG22	2:D:169:GLU:CG	2.14	0.77
2:D:31:TYR:HD1	2:D:35:ASP:HB2	1.50	0.77
1:C:142:GLU:OE1	1:C:142:GLU:N	2.17	0.75
1:C:98:ILE:H	1:C:158:PRO:HB3	1.51	0.75
1:C:95:ASP:HB3	1:C:156:ASN:HB3	1.69	0.75
2:D:7:ILE:HD11	2:D:30:LEU:HD13	1.67	0.75
1:C:67:GLY:HA3	2:D:59:VAL:HG21	1.67	0.75
1:A:20:PHE:CE2	1:A:72:VAL:HB	2.21	0.74
1:C:30:GLY:O	1:C:33:ARG:HG2	1.88	0.74
1:A:151:LEU:HD23	1:A:155:THR:OG1	1.88	0.73
1:C:87:LEU:HD23	1:C:91:ASN:HD22	1.52	0.73
1:A:155:THR:HG22	1:A:157:ARG:HB2	1.73	0.71
1:C:62:SER:O	1:C:66:LEU:HD12	1.91	0.70
2:B:78:MET:HE3	2:D:78:MET:HE3	1.73	0.70
1:C:135:GLU:N	1:C:135:GLU:OE1	2.25	0.70
2:D:168:GLN:HA	2:D:171:VAL:HG12	1.74	0.69
2:D:35:ASP:OD1	2:D:173:ARG:NH2	2.21	0.69
2:D:166:THR:HG22	2:D:169:GLU:HG3	1.73	0.69
2:D:36:ARG:HG2	2:D:38:ARG:HG2	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:SER:HB3	2:B:83:MET:HE1	1.75	0.68
1:A:13:THR:HG21	1:A:44:GLN:NE2	2.10	0.67
1:C:21:THR:HG21	1:C:60:VAL:HG23	1.78	0.66
2:D:40:PHE:HB2	2:D:174:PHE:CE2	2.31	0.66
1:A:58:LEU:HA	1:A:73:MET:HE2	1.78	0.64
2:D:98:ASP:OD2	2:D:151:LYS:NZ	2.31	0.64
2:D:4:HIS:HB3	2:D:33:ILE:HD11	1.79	0.64
2:B:3:LYS:NZ	4:B:301:HOH:O	2.21	0.64
1:C:133:TYR:HB2	1:C:162:LEU:HD11	1.80	0.64
1:C:65:TYR:CD2	1:C:96:ILE:HG23	2.34	0.63
1:A:72:VAL:HG13	1:A:99:LEU:O	1.99	0.63
2:D:38:ARG:NH1	2:D:177:GLU:OE2	2.27	0.63
1:A:155:THR:CG2	1:A:157:ARG:HB2	2.29	0.62
1:C:14:GLU:OE2	1:C:14:GLU:N	2.33	0.61
2:B:1:MET:HG3	2:B:5:ASP:HB2	1.82	0.61
1:A:163:ILE:HG22	1:A:164:LYS:HG3	1.82	0.60
1:C:155:THR:HG23	1:C:157:ARG:HB2	1.82	0.60
1:C:149:LEU:O	1:C:153:GLU:HG3	2.01	0.60
2:D:168:GLN:HA	2:D:171:VAL:CG1	2.33	0.59
1:A:36:GLU:OE1	2:D:109:ARG:HA	2.03	0.59
2:B:51:PRO:HG3	2:B:80:ILE:HD13	1.85	0.59
1:C:13:THR:OG1	1:C:14:GLU:OE2	2.17	0.59
1:A:13:THR:HG21	1:A:44:GLN:HE21	1.68	0.58
1:A:8:MET:HG3	1:A:12:LEU:HD11	1.85	0.58
2:D:20:VAL:HA	2:D:40:PHE:HB3	1.86	0.58
1:C:149:LEU:HA	1:C:152:ILE:HD12	1.86	0.58
2:B:80:ILE:HD12	2:B:83:MET:HE3	1.84	0.58
1:C:38:LYS:HZ1	1:C:44:GLN:HG3	1.69	0.58
2:D:10:ILE:CD1	2:D:95:VAL:HG21	2.33	0.58
2:B:29:ASP:O	2:B:33:ILE:HG12	2.03	0.58
1:A:72:VAL:CG2	1:A:99:LEU:HB3	2.30	0.58
2:D:165:TRP:CD1	2:D:169:GLU:OE1	2.57	0.58
1:C:133:TYR:HA	1:C:160:ALA:O	2.05	0.57
2:D:3:LYS:O	2:D:7:ILE:HG22	2.05	0.57
2:B:62:ASP:OD1	2:B:62:ASP:N	2.38	0.57
1:C:136:LEU:HD13	1:C:163:ILE:HG23	1.87	0.57
1:C:30:GLY:HA2	1:C:33:ARG:HD2	1.88	0.56
1:C:65:TYR:CZ	1:C:97:PRO:HD2	2.41	0.56
2:B:35:ASP:OD2	2:B:165:TRP:NE1	2.37	0.56
2:D:18:TYR:HD2	2:D:63:VAL:HG21	1.69	0.56
2:D:30:LEU:HG	2:D:41:TYR:OH	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:166:THR:HG22	2:D:169:GLU:HG2	1.85	0.56
2:D:66:VAL:HG12	2:D:93:ILE:HB	1.87	0.56
1:C:20:PHE:CG	1:C:72:VAL:HG22	2.41	0.56
1:C:151:LEU:O	1:C:155:THR:HG22	2.06	0.55
1:C:75:MET:HE1	1:C:83:CYS:SG	2.47	0.55
1:C:146:LEU:HA	1:C:149:LEU:HB2	1.88	0.55
1:A:145:ILE:HG22	1:A:161:ILE:HD13	1.89	0.55
1:C:65:TYR:HA	1:C:69:ARG:O	2.07	0.55
1:C:58:LEU:HD23	1:C:83:CYS:HB2	1.89	0.55
1:C:121:LYS:O	1:C:124:ASP:HB2	2.07	0.54
2:D:18:TYR:CD2	2:D:63:VAL:HG21	2.42	0.54
2:D:164:HIS:O	2:D:165:TRP:CD1	2.60	0.54
2:D:171:VAL:O	2:D:175:THR:HG22	2.08	0.54
1:A:19:HIS:HD2	1:A:64:MET:HE2	1.73	0.53
1:C:58:LEU:HD11	1:C:91:ASN:HD21	1.74	0.53
1:A:121:LYS:HG2	1:A:122:LEU:N	2.24	0.53
1:A:17:TYR:OH	1:A:152:ILE:HD11	2.08	0.53
1:A:148:ALA:O	1:A:152:ILE:HG23	2.09	0.53
1:A:16:ASN:HB3	1:A:70:LYS:HE3	1.91	0.52
2:D:10:ILE:HD11	2:D:66:VAL:HG21	1.92	0.52
1:A:30:GLY:O	1:A:33:ARG:HB2	2.09	0.52
2:D:41:TYR:HB2	2:D:170:ILE:HD13	1.92	0.52
1:C:136:LEU:CD1	1:C:163:ILE:HG23	2.40	0.52
1:C:23:VAL:HG11	1:C:53:ARG:HA	1.91	0.51
1:C:77:ASN:HB2	1:C:104:TRP:HB3	1.91	0.51
1:A:132:PRO:HG2	1:A:159:VAL:HG22	1.93	0.51
2:B:99:ASN:HB2	2:B:154:PRO:HD3	1.91	0.51
2:B:118:ASP:O	2:B:122:GLN:HG2	2.10	0.51
1:C:136:LEU:HD22	1:C:163:ILE:HA	1.92	0.51
1:C:19:HIS:C	1:C:20:PHE:HD1	2.19	0.51
1:C:38:LYS:NZ	1:C:44:GLN:HG3	2.25	0.51
1:C:59:GLY:HA3	2:D:51:PRO:HB2	1.93	0.50
2:D:27:SER:O	2:D:41:TYR:HE1	1.94	0.50
2:B:71:ASP:OD1	2:B:71:ASP:N	2.44	0.50
1:A:3:SER:OG	1:A:4:THR:N	2.41	0.50
2:B:80:ILE:HD12	2:B:83:MET:CE	2.41	0.50
2:B:181:GLU:HA	2:B:181:GLU:OE1	2.10	0.50
1:C:145:ILE:O	1:C:148:ALA:HB3	2.12	0.50
2:B:79:GLY:HA2	2:D:78:MET:HE2	1.94	0.50
1:A:3:SER:O	1:A:6:GLU:HG2	2.12	0.49
1:A:51:SER:HA	2:B:83:MET:SD	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:118:ASP:O	2:D:122:GLN:HG2	2.11	0.49
2:B:130:GLU:OE2	2:B:132:ASN:ND2	2.46	0.49
2:B:171:VAL:O	2:B:175:THR:HG22	2.12	0.49
1:C:90:PHE:HB2	2:D:45:SER:OG	2.12	0.48
1:C:9:LEU:O	1:C:13:THR:HG23	2.13	0.48
1:A:10:SER:O	1:A:13:THR:HG22	2.13	0.48
1:A:70:LYS:H	1:A:70:LYS:HE2	1.79	0.48
1:A:126:LEU:O	1:A:130:ASP:N	2.47	0.47
1:C:119:GLY:O	1:C:123:THR:HG23	2.14	0.47
2:D:27:SER:HB3	2:D:41:TYR:HD1	1.78	0.47
2:D:78:MET:O	2:D:81:ILE:HG12	2.14	0.47
1:A:8:MET:O	1:A:12:LEU:HD12	2.14	0.47
1:C:161:ILE:HG13	1:C:163:ILE:HD11	1.96	0.47
2:D:7:ILE:HA	2:D:10:ILE:CG2	2.40	0.47
2:B:63:VAL:CG1	2:B:182:ASN:HD21	2.28	0.47
2:D:21:SER:HA	2:D:68:LEU:HB2	1.96	0.47
1:C:74:LEU:HG	1:C:101:LEU:HD21	1.96	0.47
2:B:155:ARG:HH21	2:B:155:ARG:HG3	1.78	0.47
2:B:166:THR:HG23	2:B:169:GLU:H	1.79	0.47
1:C:148:ALA:HA	1:C:159:VAL:HG21	1.96	0.47
1:C:149:LEU:O	1:C:152:ILE:HB	2.14	0.47
2:D:76:MET:HE3	2:D:76:MET:HB2	1.85	0.47
1:A:36:GLU:OE1	2:D:109:ARG:CA	2.63	0.47
1:A:59:GLY:HA3	2:B:51:PRO:HB2	1.97	0.47
1:C:136:LEU:O	1:C:136:LEU:HD23	2.15	0.47
1:C:154:LYS:C	1:C:154:LYS:HD3	2.40	0.46
1:A:155:THR:HG22	1:A:157:ARG:HD2	1.96	0.46
1:C:144:THR:O	1:C:148:ALA:CB	2.64	0.46
2:D:14:PHE:HB3	2:D:17:ALA:HB2	1.97	0.46
2:D:166:THR:N	2:D:169:GLU:HG3	2.31	0.46
2:B:79:GLY:O	2:B:82:THR:OG1	2.29	0.46
2:B:109:ARG:HG2	2:B:110:THR:HG22	1.97	0.46
2:D:18:TYR:HD2	2:D:63:VAL:CG2	2.29	0.46
1:C:101:LEU:HB2	1:C:163:ILE:CD1	2.46	0.46
1:A:31:PHE:N	1:A:31:PHE:CD2	2.83	0.46
1:C:121:LYS:H	1:C:121:LYS:CD	2.17	0.46
2:D:88:LYS:O	2:D:90:LYS:HE2	2.16	0.46
1:A:65:TYR:CZ	1:A:97:PRO:HD2	2.50	0.45
2:D:31:TYR:OH	2:D:164:HIS:NE2	2.39	0.45
1:A:36:GLU:OE1	2:D:109:ARG:N	2.50	0.45
2:B:164:HIS:O	2:B:164:HIS:ND1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:ASN:HD21	1:C:69:ARG:HH12	1.65	0.45
1:C:77:ASN:OD1	1:C:122:LEU:HD22	2.17	0.45
2:D:30:LEU:HD11	2:D:39:ASN:OD1	2.17	0.45
2:D:60:TYR:HB3	2:D:63:VAL:HG12	1.99	0.45
1:A:75:MET:HE1	1:A:80:LEU:HA	1.99	0.45
1:C:19:HIS:C	1:C:20:PHE:CD1	2.94	0.45
1:C:32:PHE:O	1:C:36:GLU:HG3	2.16	0.45
1:A:65:TYR:CD2	1:A:96:ILE:HG23	2.52	0.45
1:C:83:CYS:O	1:C:86:VAL:HG22	2.18	0.44
2:D:57:SER:OG	2:D:65:LEU:HD11	2.18	0.44
1:C:155:THR:HG23	1:C:157:ARG:N	2.33	0.44
1:C:155:THR:O	1:C:156:ASN:HB2	2.17	0.44
1:A:145:ILE:HA	1:A:161:ILE:HD11	2.00	0.44
1:C:19:HIS:HB3	1:C:64:MET:CE	2.48	0.44
1:C:28:LEU:HD13	1:C:74:LEU:HD23	2.00	0.44
1:C:137:ASP:OD1	1:C:137:ASP:N	2.50	0.44
2:D:31:TYR:CD2	2:D:163:VAL:HG23	2.53	0.44
1:A:24:PRO:HB3	2:D:109:ARG:NH2	2.17	0.44
2:D:48:MET:C	2:D:51:PRO:HD2	2.43	0.43
1:C:92:PHE:CD2	1:C:157:ARG:HG2	2.53	0.43
2:D:37:ALA:HA	2:D:173:ARG:NH2	2.33	0.43
2:D:55:GLY:O	2:D:59:VAL:HG22	2.19	0.43
2:D:36:ARG:CG	2:D:38:ARG:HG2	2.44	0.43
2:B:176:ASN:O	2:B:180:LEU:HG	2.19	0.43
1:C:141:SER:O	1:C:145:ILE:HG13	2.19	0.43
2:D:18:TYR:CD1	2:D:38:ARG:CB	2.95	0.43
2:B:48:MET:C	2:B:51:PRO:HD2	2.44	0.43
1:A:101:LEU:HD23	1:A:161:ILE:HB	2.01	0.43
2:D:94:HIS:O	2:D:147:LEU:HA	2.19	0.42
1:C:133:TYR:HB2	1:C:162:LEU:CD1	2.49	0.42
2:D:68:LEU:HD12	2:D:97:LEU:HD11	2.01	0.42
1:A:58:LEU:HB2	1:A:73:MET:HE1	2.00	0.42
1:C:94:TYR:HB3	1:C:96:ILE:HD11	2.00	0.42
1:A:92:PHE:HE2	1:A:130:ASP:O	2.01	0.42
1:A:65:TYR:HA	1:A:69:ARG:O	2.19	0.42
2:B:9:LEU:HD21	2:B:138:PHE:CZ	2.55	0.42
2:D:172:GLN:HG3	2:D:173:ARG:H	1.83	0.42
2:D:50:ALA:HB3	2:D:51:PRO:HD3	2.00	0.42
1:A:149:LEU:O	1:A:152:ILE:HG12	2.20	0.42
2:B:77:ASN:O	2:B:80:ILE:HG22	2.20	0.42
1:C:23:VAL:HG11	1:C:53:ARG:CA	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:PRO:HB2	1:A:159:VAL:HG13	2.02	0.41
2:B:64:PRO:HA	2:B:91:ASN:HB3	2.02	0.41
2:D:36:ARG:HG3	2:D:37:ALA:N	2.34	0.41
2:D:31:TYR:CG	2:D:163:VAL:HG23	2.55	0.41
1:A:58:LEU:CA	1:A:73:MET:HE2	2.47	0.41
2:D:10:ILE:HG21	2:D:10:ILE:HD13	1.78	0.41
1:A:25:CYS:O	1:A:29:LYS:HD3	2.21	0.41
1:C:121:LYS:HD3	1:C:121:LYS:N	2.19	0.41
2:D:161:LYS:HD3	2:D:162:ARG:O	2.21	0.41
1:A:151:LEU:HD23	1:A:155:THR:HG1	1.84	0.40
1:A:92:PHE:CE1	1:A:158:PRO:HG2	2.56	0.40
1:A:145:ILE:O	1:A:149:LEU:HG	2.21	0.40
1:A:64:MET:HG2	2:B:59:VAL:HG23	2.02	0.40
1:A:125:LEU:O	1:A:129:VAL:HG22	2.22	0.40
1:A:136:LEU:HD11	1:A:141:SER:HA	2.04	0.40
1:A:145:ILE:HG13	1:A:146:LEU:N	2.36	0.40
2:D:36:ARG:HG3	2:D:38:ARG:H	1.86	0.40
2:D:168:GLN:O	2:D:172:GLN:HG2	2.20	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	136/181 (75%)	128 (94%)	8 (6%)	0	100	100
1	C	138/181 (76%)	130 (94%)	8 (6%)	0	100	100
2	B	168/186 (90%)	164 (98%)	4 (2%)	0	100	100
2	D	166/186 (89%)	156 (94%)	10 (6%)	0	100	100
All	All	608/734 (83%)	578 (95%)	30 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	127/160 (79%)	127 (100%)	0	100	100
1	C	129/160 (81%)	129 (100%)	0	100	100
2	B	151/161 (94%)	151 (100%)	0	100	100
2	D	149/161 (92%)	149 (100%)	0	100	100
All	All	556/642 (87%)	556 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
2	B	32	ASN
2	B	182	ASN
1	C	15	ASN
1	C	45	ASN
1	C	76	GLN
1	C	91	ASN
2	D	2	ASN
2	D	25	HIS
2	D	86	HIS

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](#)

7 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	$\# Z > 2$
3	SO4	D	203	-	4,4,4	0.24	0	6,6,6	0.05	0
3	SO4	B	204	-	4,4,4	0.24	0	6,6,6	0.13	0
3	SO4	B	202	-	4,4,4	0.24	0	6,6,6	0.09	0
3	SO4	B	201	-	4,4,4	0.21	0	6,6,6	0.15	0
3	SO4	B	203	-	4,4,4	0.24	0	6,6,6	0.10	0
3	SO4	D	201	-	4,4,4	0.25	0	6,6,6	0.06	0
3	SO4	D	202	-	4,4,4	0.24	0	6,6,6	0.08	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	142/181 (78%)	1.92	60 (42%) 0 0	55, 107, 181, 211	0
1	C	144/181 (79%)	2.11	69 (47%) 0 0	63, 111, 164, 213	0
2	B	174/186 (93%)	0.61	17 (9%) 13 11	39, 61, 137, 189	0
2	D	172/186 (92%)	1.34	50 (29%) 1 1	42, 93, 171, 216	0
All	All	632/734 (86%)	1.45	196 (31%) 1 1	39, 92, 171, 216	0

All (196) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	21	SER	6.9
1	C	119	GLY	6.6
1	C	136	LEU	5.9
1	A	27	LEU	5.7
2	B	159	ILE	5.6
1	A	5	ALA	5.4
1	C	32	PHE	5.2
2	D	159	ILE	5.2
2	B	184	VAL	5.2
1	C	144	THR	5.1
1	A	20	PHE	5.1
1	C	82	TYR	4.9
1	A	31	PHE	4.8
1	A	26	SER	4.8
1	C	104	TRP	4.8
2	B	165	TRP	4.7
1	A	145	ILE	4.6
2	D	26	ILE	4.6
1	A	35	LEU	4.6
1	A	159	VAL	4.5
1	A	103	SER	4.5

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Mol	Chain	Res	Type	RSRZ
2	B	138	PHE	4.5
1	A	119	GLY	4.4
1	A	150	PHE	4.4
2	D	180	LEU	4.4
1	C	38	LYS	4.3
1	A	102	ILE	4.3
2	D	163	VAL	4.3
1	C	20	PHE	4.3
1	A	9	LEU	4.3
1	A	74	LEU	4.2
1	C	45	ASN	4.2
1	A	164	LYS	4.1
2	D	154	PRO	4.1
2	D	18	TYR	4.0
2	D	165	TRP	4.0
2	D	65	LEU	4.0
1	A	71	CYS	4.0
2	B	180	LEU	3.9
1	A	8	MET	3.9
2	D	134	GLY	3.9
2	D	174	PHE	3.8
1	C	135	GLU	3.8
2	D	170	ILE	3.7
2	B	163	VAL	3.7
2	D	109	ARG	3.7
1	C	44	GLN	3.6
1	C	77	ASN	3.6
1	C	93	ILE	3.6
1	A	38	LYS	3.5
1	C	162	LEU	3.5
1	C	150	PHE	3.5
1	A	101	LEU	3.4
1	C	71	CYS	3.4
1	C	5	ALA	3.4
1	C	161	ILE	3.4
1	A	7	ARG	3.4
1	A	141	SER	3.4
1	A	34	LEU	3.3
1	C	101	LEU	3.3
1	C	31	PHE	3.3
1	A	161	ILE	3.3
2	B	134	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
2	D	101	MET	3.3
1	A	134	LYS	3.3
1	C	9	LEU	3.3
2	D	167	PRO	3.2
1	C	164	LYS	3.2
1	C	46	ILE	3.2
2	D	40	PHE	3.2
1	C	94	TYR	3.2
1	C	99	LEU	3.2
2	B	142	ASN	3.2
1	A	82	TYR	3.2
1	C	88	THR	3.2
1	C	102	ILE	3.2
1	C	138	TYR	3.1
1	C	35	LEU	3.1
1	A	138	TYR	3.1
1	C	133	TYR	3.1
2	D	60	TYR	3.1
1	C	68	GLY	3.1
2	D	41	TYR	3.0
1	C	152	ILE	3.0
1	A	4	THR	3.0
1	C	17	TYR	3.0
1	A	12	LEU	3.0
1	A	23	VAL	3.0
1	C	145	ILE	3.0
1	A	151	LEU	3.0
1	A	44	GLN	3.0
1	C	8	MET	2.9
2	D	17	ALA	2.9
1	C	28	LEU	2.9
2	B	101	MET	2.9
1	C	146	LEU	2.9
1	C	163	ILE	2.9
2	B	136	LYS	2.9
2	D	171	VAL	2.9
1	A	144	THR	2.9
2	D	11	LEU	2.8
1	C	151	LEU	2.8
1	A	92	PHE	2.8
2	D	179	THR	2.8
1	A	85	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	132	PRO	2.8
1	C	66	LEU	2.8
1	C	27	LEU	2.7
1	A	70	LYS	2.7
1	A	25	CYS	2.7
1	A	28	LEU	2.7
2	B	164	HIS	2.7
1	C	92	PHE	2.7
1	C	159	VAL	2.7
2	D	19	LEU	2.7
1	C	97	PRO	2.7
2	D	32	ASN	2.7
1	C	100	LEU	2.7
1	A	155	THR	2.7
2	D	100	GLY	2.6
1	C	70	LYS	2.6
1	A	72	VAL	2.6
1	A	148	ALA	2.6
2	D	172	GLN	2.6
1	C	7	ARG	2.6
1	A	32	PHE	2.6
1	C	72	VAL	2.6
1	A	13	THR	2.6
1	C	4	THR	2.6
1	A	99	LEU	2.6
1	C	156	ASN	2.6
2	D	137	SER	2.6
2	D	43	VAL	2.5
2	B	109	ARG	2.5
1	A	131	ILE	2.5
2	D	99	ASN	2.5
2	D	22	THR	2.5
1	A	143	GLY	2.5
1	A	152	ILE	2.5
1	C	122	LEU	2.5
2	D	138	PHE	2.5
1	A	46	ILE	2.5
1	A	121	LYS	2.5
2	D	38	ARG	2.5
1	C	160	ALA	2.5
1	C	126	LEU	2.4
1	A	16	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	129	VAL	2.4
2	B	183	GLU	2.4
1	C	67	GLY	2.4
1	A	142	GLU	2.4
1	C	12	LEU	2.4
2	D	15	PRO	2.3
1	A	10	SER	2.3
1	C	30	GLY	2.3
1	A	160	ALA	2.3
1	C	148	ALA	2.3
2	D	183	GLU	2.3
1	C	26	SER	2.3
2	D	31	TYR	2.3
2	B	181	GLU	2.3
1	C	103	SER	2.3
1	C	37	SER	2.3
2	B	154	PRO	2.3
1	A	36	GLU	2.2
1	C	125	LEU	2.2
1	C	3	SER	2.2
2	D	20	VAL	2.2
2	B	182	ASN	2.2
2	D	39	ASN	2.2
2	D	4	HIS	2.2
2	D	25	HIS	2.2
1	A	84	LEU	2.2
2	D	178	LEU	2.2
2	D	62	ASP	2.2
2	D	151	LYS	2.2
1	C	80	LEU	2.2
2	D	7	ILE	2.2
2	D	8	GLN	2.1
1	C	131	ILE	2.1
1	C	129	VAL	2.1
1	C	34	LEU	2.1
2	D	33	ILE	2.1
1	C	78	SER	2.1
2	B	62	ASP	2.1
2	D	45	SER	2.1
1	C	15	ASN	2.1
1	C	143	GLY	2.1
1	A	147	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	80	LEU	2.0
1	A	125	LEU	2.0
2	D	176	ASN	2.0
2	D	110	THR	2.0
1	A	17	TYR	2.0
2	D	13	GLN	2.0
2	D	166	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 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
3	SO4	D	203	5/5	0.71	0.14	169,172,175,176	0
3	SO4	B	203	5/5	0.76	0.18	132,134,140,155	0
3	SO4	B	202	5/5	0.85	0.15	73,94,118,119	0
3	SO4	B	204	5/5	0.87	0.11	99,112,122,128	0
3	SO4	D	201	5/5	0.89	0.10	106,108,116,123	0
3	SO4	D	202	5/5	0.90	0.10	95,104,116,125	0
3	SO4	B	201	5/5	0.99	0.05	59,60,67,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.