



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 09:31 AM EDT

PDB ID : 3FDU / pdb_00003fd
Title : Crystal structure of a putative enoyl-CoA hydratase/isomerase from *Acinetobacter baumannii*
Authors : Bonanno, J.B.; Dickey, M.; Bain, K.T.; Tang, B.K.; Romero, R.; Wasserman, S.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2008-11-26
Resolution : 2.00 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

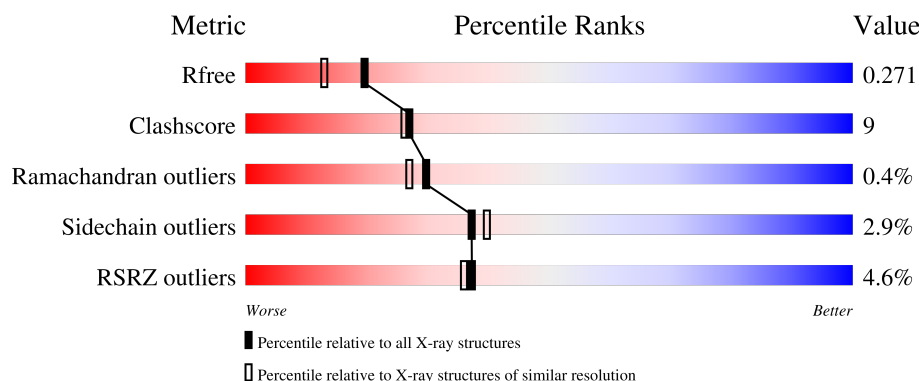
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	266	83% 10% 7%
1	B	266	7% 72% 14% 13%
1	C	266	3% 71% 13% 15%
1	D	266	3% 71% 12% 15%

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Mol	Chain	Length	Quality of chain
1	E	266	5% 76% 12% 12%
1	F	266	5% 64% 15% • 19%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11085 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 enoyl-CoA hydratase/isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	0	1	0
			1873	1202	317	347	7			
1	B	232	Total	C	N	O	S	0	0	0
			1735	1113	295	321	6			
1	C	227	Total	C	N	O	S	0	0	0
			1710	1096	291	318	5			
1	D	225	Total	C	N	O	S	0	0	0
			1690	1087	289	310	4			
1	E	234	Total	C	N	O	S	0	0	0
			1757	1128	296	327	6			
1	F	215	Total	C	N	O	S	0	0	0
			1611	1034	276	298	3			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MET	-	expression tag	UNP A3M7S1
A	8	SER	-	expression tag	UNP A3M7S1
A	9	LEU	-	expression tag	UNP A3M7S1
A	11	PRO	GLN	engineered mutation	UNP A3M7S1
A	14	ASN	GLN	engineered mutation	UNP A3M7S1
A	59	VAL	ILE	engineered mutation	UNP A3M7S1
A	259	GLN	LYS	engineered mutation	UNP A3M7S1
A	265	GLU	-	expression tag	UNP A3M7S1
A	266	GLY	-	expression tag	UNP A3M7S1
A	267	HIS	-	expression tag	UNP A3M7S1
A	268	HIS	-	expression tag	UNP A3M7S1
A	269	HIS	-	expression tag	UNP A3M7S1
A	270	HIS	-	expression tag	UNP A3M7S1
A	271	HIS	-	expression tag	UNP A3M7S1
A	272	HIS	-	expression tag	UNP A3M7S1
B	7	MET	-	expression tag	UNP A3M7S1
B	8	SER	-	expression tag	UNP A3M7S1

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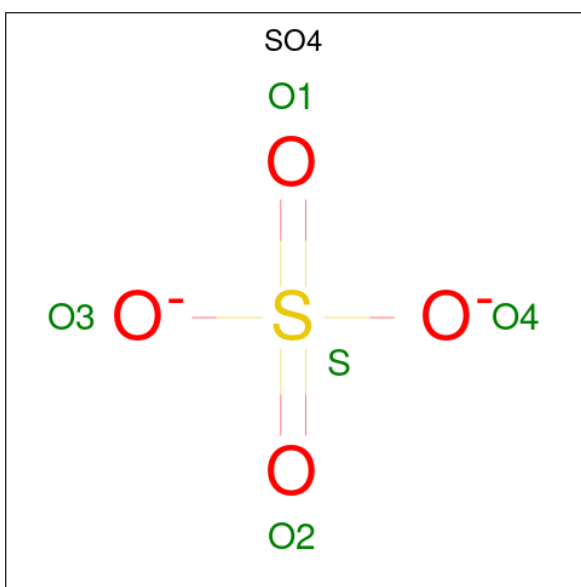
Chain	Residue	Modelled	Actual	Comment	Reference
B	9	LEU	-	expression tag	UNP A3M7S1
B	11	PRO	GLN	engineered mutation	UNP A3M7S1
B	14	ASN	GLN	engineered mutation	UNP A3M7S1
B	59	VAL	ILE	engineered mutation	UNP A3M7S1
B	259	GLN	LYS	engineered mutation	UNP A3M7S1
B	265	GLU	-	expression tag	UNP A3M7S1
B	266	GLY	-	expression tag	UNP A3M7S1
B	267	HIS	-	expression tag	UNP A3M7S1
B	268	HIS	-	expression tag	UNP A3M7S1
B	269	HIS	-	expression tag	UNP A3M7S1
B	270	HIS	-	expression tag	UNP A3M7S1
B	271	HIS	-	expression tag	UNP A3M7S1
B	272	HIS	-	expression tag	UNP A3M7S1
C	7	MET	-	expression tag	UNP A3M7S1
C	8	SER	-	expression tag	UNP A3M7S1
C	9	LEU	-	expression tag	UNP A3M7S1
C	11	PRO	GLN	engineered mutation	UNP A3M7S1
C	14	ASN	GLN	engineered mutation	UNP A3M7S1
C	59	VAL	ILE	engineered mutation	UNP A3M7S1
C	259	GLN	LYS	engineered mutation	UNP A3M7S1
C	265	GLU	-	expression tag	UNP A3M7S1
C	266	GLY	-	expression tag	UNP A3M7S1
C	267	HIS	-	expression tag	UNP A3M7S1
C	268	HIS	-	expression tag	UNP A3M7S1
C	269	HIS	-	expression tag	UNP A3M7S1
C	270	HIS	-	expression tag	UNP A3M7S1
C	271	HIS	-	expression tag	UNP A3M7S1
C	272	HIS	-	expression tag	UNP A3M7S1
D	7	MET	-	expression tag	UNP A3M7S1
D	8	SER	-	expression tag	UNP A3M7S1
D	9	LEU	-	expression tag	UNP A3M7S1
D	11	PRO	GLN	engineered mutation	UNP A3M7S1
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D	266	GLY	-	expression tag	UNP A3M7S1
D	267	HIS	-	expression tag	UNP A3M7S1
D	268	HIS	-	expression tag	UNP A3M7S1
D	269	HIS	-	expression tag	UNP A3M7S1
D	270	HIS	-	expression tag	UNP A3M7S1
D	271	HIS	-	expression tag	UNP A3M7S1

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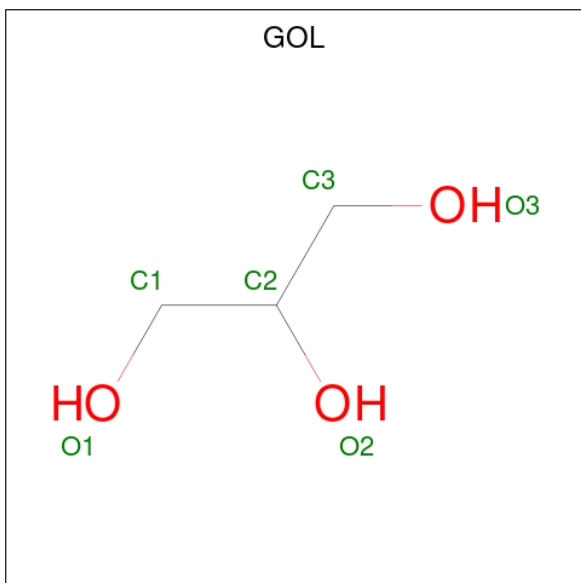
Chain	Residue	Modelled	Actual	Comment	Reference
D	272	HIS	-	expression tag	UNP A3M7S1
E	7	MET	-	expression tag	UNP A3M7S1
E	8	SER	-	expression tag	UNP A3M7S1
E	9	LEU	-	expression tag	UNP A3M7S1
E	11	PRO	GLN	engineered mutation	UNP A3M7S1
E	14	ASN	GLN	engineered mutation	UNP A3M7S1
E	59	VAL	ILE	engineered mutation	UNP A3M7S1
E	259	GLN	LYS	engineered mutation	UNP A3M7S1
E	265	GLU	-	expression tag	UNP A3M7S1
E	266	GLY	-	expression tag	UNP A3M7S1
E	267	HIS	-	expression tag	UNP A3M7S1
E	268	HIS	-	expression tag	UNP A3M7S1
E	269	HIS	-	expression tag	UNP A3M7S1
E	270	HIS	-	expression tag	UNP A3M7S1
E	271	HIS	-	expression tag	UNP A3M7S1
E	272	HIS	-	expression tag	UNP A3M7S1
F	7	MET	-	expression tag	UNP A3M7S1
F	8	SER	-	expression tag	UNP A3M7S1
F	9	LEU	-	expression tag	UNP A3M7S1
F	11	PRO	GLN	engineered mutation	UNP A3M7S1
F	14	ASN	GLN	engineered mutation	UNP A3M7S1
F	59	VAL	ILE	engineered mutation	UNP A3M7S1
F	259	GLN	LYS	engineered mutation	UNP A3M7S1
F	265	GLU	-	expression tag	UNP A3M7S1
F	266	GLY	-	expression tag	UNP A3M7S1
F	267	HIS	-	expression tag	UNP A3M7S1
F	268	HIS	-	expression tag	UNP A3M7S1
F	269	HIS	-	expression tag	UNP A3M7S1
F	270	HIS	-	expression tag	UNP A3M7S1
F	271	HIS	-	expression tag	UNP A3M7S1
F	272	HIS	-	expression tag	UNP A3M7S1

- 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	C	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		

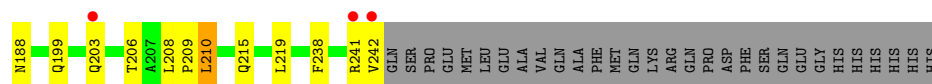
- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



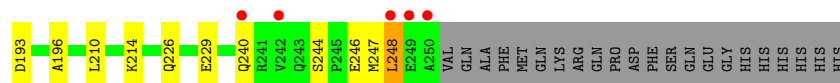
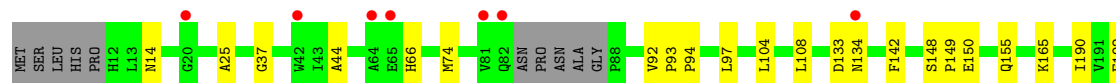
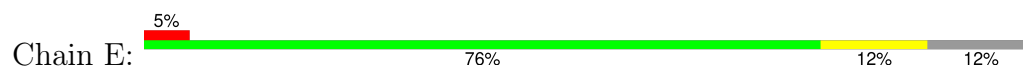
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

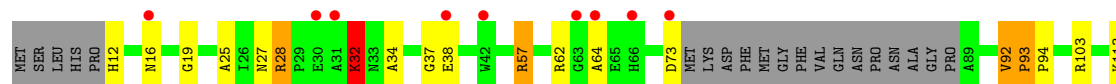
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	144	Total	O	0	0
			144	144		
4	B	116	Total	O	0	0
			116	116		
4	C	112	Total	O	0	0
			112	112		
4	D	120	Total	O	0	0
			120	120		
4	E	97	Total	O	0	0
			97	97		
4	F	94	Total	O	0	0
			94	94		



- Molecule 1: Putative enoyl-CoA hydratase/isomerase



- Molecule 1: Putative enoyl-CoA hydratase/isomerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.58Å 71.73Å 132.88Å 90.00° 91.36° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.1 (20.00-2.00) 98.7 (20.00-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.90 (at 2.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.226 , 0.283 0.219 , 0.271	Depositor DCC
R_{free} test set	5421 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.590	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 54.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11085	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.01% 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: SO4, GOL

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	1.14	1/1910 (0.1%)	0.99	1/2596 (0.0%)
1	B	0.90	1/1765 (0.1%)	0.95	1/2400 (0.0%)
1	C	1.00	1/1739 (0.1%)	0.97	1/2363 (0.0%)
1	D	0.89	0/1719	0.98	5/2336 (0.2%)
1	E	0.84	0/1786	0.95	3/2425 (0.1%)
1	F	0.83	0/1636	0.98	5/2223 (0.2%)
All	All	0.94	3/10555 (0.0%)	0.97	16/14343 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	93	PRO	CA-C	6.82	1.58	1.52
1	A	92	VAL	CA-C	5.15	1.57	1.52
1	B	218	ALA	CA-CB	5.09	1.61	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	92	VAL	CA-C-N	8.61	129.25	120.38
1	F	92	VAL	C-N-CA	8.61	129.25	120.38
1	F	28	ARG	CA-C-N	7.98	128.16	119.87
1	F	28	ARG	C-N-CA	7.98	128.16	119.87
1	D	93	PRO	N-CA-C	7.87	120.30	110.70
1	B	93	PRO	N-CA-C	6.75	118.94	110.70
1	C	93	PRO	N-CA-C	6.48	118.61	110.70
1	E	93	PRO	N-CA-C	6.43	118.55	110.70
1	E	244	SER	CA-C-N	6.23	125.96	119.05
1	E	244	SER	C-N-CA	6.23	125.96	119.05
1	A	93	PRO	N-CA-C	5.92	117.93	110.70
1	D	188	ASN	N-CA-C	5.30	117.14	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	93	PRO	CA-C-N	-5.25	113.50	119.28
1	D	93	PRO	C-N-CA	-5.25	113.50	119.28
1	F	93	PRO	N-CA-C	5.23	117.08	110.70
1	D	177	ASN	N-CA-C	5.08	117.91	109.94

There are no chirality outliers.

There are no planarity outliers.

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	1873	0	1895	16	0
1	B	1735	0	1747	62	0
1	C	1710	0	1740	39	0
1	D	1690	0	1723	27	0
1	E	1757	0	1778	19	2
1	F	1611	0	1644	36	0
2	A	5	0	0	1	0
2	C	5	0	0	0	0
2	E	10	0	0	0	0
3	A	6	0	8	0	0
4	A	144	0	0	1	0
4	B	116	0	0	4	0
4	C	112	0	0	2	1
4	D	120	0	0	3	0
4	E	97	0	0	5	0
4	F	94	0	0	6	1
All	All	11085	0	10535	192	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 9.

All (192) 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:B:77:PHE:CZ	1:B:247:MET:HE1	1.58	1.37
1:B:77:PHE:HZ	1:B:247:MET:CE	1.34	1.37
1:C:9:LEU:HD23	1:C:10:HIS:N	1.38	1.35
1:B:77:PHE:CZ	1:B:247:MET:CE	2.15	1.24
1:B:239:MET:CE	1:B:239:MET:HA	1.71	1.20
1:B:74:MET:HE2	1:B:77:PHE:CD2	1.79	1.18
1:C:92:VAL:HG11	1:C:239:MET:CE	1.77	1.13
1:C:95:PHE:HE2	1:C:239:MET:HE2	1.10	1.12
1:B:239:MET:HE1	1:B:242:VAL:HG21	1.16	1.11
1:B:16:ASN:HD22	1:B:17:LEU:N	1.52	1.08
1:B:239:MET:HA	1:B:239:MET:HE2	1.32	1.07
1:D:74:MET:HE1	4:D:281:HOH:O	1.57	1.04
1:C:92:VAL:HG11	1:C:239:MET:HE1	1.38	1.03
1:C:9:LEU:CD2	1:C:10:HIS:H	1.72	1.02
1:B:16:ASN:HD22	1:B:16:ASN:C	1.69	0.99
1:B:77:PHE:HZ	1:B:247:MET:HE1	0.90	0.98
1:B:77:PHE:CZ	1:B:247:MET:HE2	1.99	0.98
1:C:92:VAL:HG21	1:C:239:MET:HE3	1.46	0.96
1:B:239:MET:CE	1:B:242:VAL:HG21	1.95	0.95
1:C:95:PHE:CE2	1:C:239:MET:HE2	2.02	0.94
1:B:239:MET:HE1	1:B:242:VAL:CG2	1.96	0.94
1:F:113:LYS:HD2	1:F:195:TYR:CZ	2.04	0.93
1:C:9:LEU:CD2	1:C:10:HIS:N	2.29	0.91
1:B:189:GLU:HB2	4:B:279:HOH:O	1.69	0.90
1:C:92:VAL:HG11	1:C:239:MET:HE3	1.56	0.87
1:F:203:GLN:HG2	4:F:927:HOH:O	1.72	0.87
1:B:243:GLN:O	1:B:243:GLN:CG	2.23	0.86
1:B:239:MET:HA	1:B:239:MET:HE3	1.56	0.85
1:B:239:MET:CE	1:B:242:VAL:CG2	2.54	0.84
1:B:77:PHE:CE2	1:B:247:MET:HE1	2.11	0.84
1:F:32:LYS:HE3	4:F:931:HOH:O	1.80	0.81
1:B:65:GLU:HG2	4:B:283:HOH:O	1.81	0.80
1:D:142:PHE:CE2	1:D:150:GLU:HG2	2.16	0.80
1:C:92:VAL:CG2	1:C:239:MET:HE3	2.12	0.79
1:A:41:LEU:O	1:A:45:LYS:HG2	1.83	0.78
1:B:16:ASN:C	1:B:16:ASN:ND2	2.34	0.77
1:B:73:ASP:HB3	1:B:76:ASP:HB3	1.67	0.76
1:E:66:HIS:HD2	4:E:304:HOH:O	1.68	0.76
1:B:239:MET:CE	1:B:239:MET:CA	2.60	0.74
1:B:137:LEU:C	1:B:137:LEU:HD13	2.13	0.74
1:D:74:MET:HA	1:D:74:MET:HE2	1.69	0.73
1:B:74:MET:O	1:B:77:PHE:HB3	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:VAL:CG1	1:C:239:MET:HE3	2.19	0.72
1:F:225:ASP:O	1:F:229:GLU:HG3	1.91	0.71
1:C:92:VAL:CG1	1:C:239:MET:CE	2.63	0.71
1:B:12:HIS:CD2	1:B:28:ARG:HG3	2.27	0.70
1:C:92:VAL:CB	1:C:239:MET:HE3	2.23	0.69
1:B:243:GLN:O	1:B:243:GLN:HG3	1.94	0.68
1:F:57:ARG:HD2	4:F:306:HOH:O	1.93	0.68
1:B:65:GLU:HG3	1:B:66:HIS:N	2.08	0.68
1:B:243:GLN:O	1:B:243:GLN:HG2	1.93	0.67
1:C:74:MET:HA	1:C:74:MET:HE2	1.77	0.66
1:B:77:PHE:HZ	1:B:247:MET:HE2	1.35	0.66
1:F:146:GLY:O	1:F:241:ARG:HD3	1.94	0.66
1:B:16:ASN:ND2	1:B:17:LEU:N	2.36	0.64
1:E:229:GLU:HG3	4:E:294:HOH:O	1.98	0.64
1:B:245:PRO:HD3	4:B:290:HOH:O	1.97	0.63
1:C:9:LEU:HD23	1:C:9:LEU:C	2.14	0.62
1:B:199:GLN:NE2	1:B:203:GLN:OE1	2.23	0.61
1:B:202:ALA:O	1:B:206:THR:HG23	2.01	0.60
1:F:19:GLY:O	4:F:812:HOH:O	2.16	0.60
1:D:147:LEU:HA	1:D:241:ARG:HD3	1.84	0.60
1:B:77:PHE:CE2	1:B:247:MET:CE	2.79	0.59
1:F:148:SER:HB2	1:F:149:PRO:CD	2.32	0.59
1:D:133:ASP:OD2	4:D:300:HOH:O	2.17	0.58
1:D:142:PHE:CZ	1:D:150:GLU:HG2	2.40	0.57
1:B:238:PHE:HD2	1:B:239:MET:HE3	1.70	0.57
1:A:202:ALA:O	1:A:206:THR:HG23	2.05	0.56
1:F:62:ARG:NH2	1:F:195:TYR:HB3	2.21	0.56
1:B:137:LEU:C	1:B:137:LEU:CD1	2.78	0.56
1:F:28:ARG:HG2	1:F:28:ARG:O	2.05	0.55
1:E:193:ASP:OD2	1:E:196:ALA:HB2	2.07	0.55
1:B:199:GLN:HE21	1:B:203:GLN:CD	2.13	0.54
1:C:142:PHE:CE2	1:C:150:GLU:HG2	2.41	0.54
1:B:65:GLU:HG3	1:B:66:HIS:H	1.72	0.54
1:B:74:MET:HG3	1:B:77:PHE:HD2	1.73	0.54
1:B:239:MET:HE3	1:B:239:MET:CA	2.31	0.54
1:D:146:GLY:O	1:D:241:ARG:NH2	2.40	0.54
1:B:9:LEU:HG	1:B:10:HIS:H	1.72	0.54
1:C:214:LYS:HG3	4:C:317:HOH:O	2.08	0.54
1:B:225:ASP:O	1:B:229:GLU:HG3	2.08	0.54
1:B:246:GLU:HG2	1:C:209:PRO:HB3	1.90	0.53
1:E:165:LYS:HE3	4:E:459:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:62:ARG:HH21	1:F:195:TYR:HB3	1.73	0.53
1:F:113:LYS:HD2	1:F:195:TYR:OH	2.09	0.53
1:D:119:ILE:HG13	1:D:119:ILE:O	2.09	0.53
1:F:92:VAL:HG12	1:F:94:PRO:HD2	1.89	0.53
1:D:74:MET:HA	1:D:74:MET:CE	2.35	0.53
1:E:248:LEU:HD12	4:E:645:HOH:O	2.08	0.52
1:C:16:ASN:O	1:C:22:LEU:HD12	2.10	0.52
1:D:174:LYS:NZ	4:D:504:HOH:O	2.40	0.52
1:B:74:MET:HE2	1:B:77:PHE:CG	2.37	0.52
1:D:199:GLN:HE21	1:D:203:GLN:CG	2.23	0.52
1:D:67:ASP:OD1	1:D:115:VAL:HG22	2.10	0.51
1:E:92:VAL:HG12	1:E:94:PRO:HD2	1.93	0.51
1:B:74:MET:C	1:B:77:PHE:HB3	2.35	0.51
1:E:210:LEU:HG	1:E:214:LYS:HE3	1.92	0.51
1:A:145:LEU:O	1:A:247:MET:HE1	2.11	0.50
1:B:74:MET:CE	1:B:77:PHE:CD2	2.72	0.50
1:E:14:ASN:HB2	1:E:25:ALA:HB3	1.93	0.50
1:F:103:ARG:HD2	4:F:963:HOH:O	2.12	0.50
1:A:92:VAL:HG12	1:A:94:PRO:HD2	1.94	0.49
1:C:12:HIS:HD2	1:C:36:TYR:OH	1.94	0.49
1:C:9:LEU:HD23	1:C:10:HIS:H	0.76	0.49
1:D:57:ARG:NH1	1:D:210:LEU:HB2	2.27	0.49
1:B:74:MET:HA	1:B:77:PHE:HB3	1.95	0.49
1:F:114:GLY:O	1:F:136:ALA:HA	2.13	0.49
1:E:142:PHE:CZ	1:E:150:GLU:HG2	2.47	0.49
1:F:34:ALA:HB1	1:F:73:ASP:HA	1.95	0.49
1:D:45:LYS:HE3	1:D:49:GLU:OE2	2.13	0.49
1:D:208:LEU:HB3	1:D:209:PRO:HD2	1.94	0.49
1:D:74:MET:HE2	1:D:74:MET:CA	2.42	0.48
1:C:92:VAL:HG12	1:C:94:PRO:HD2	1.95	0.48
1:E:134:ASN:OD1	1:E:190:ILE:CG2	2.61	0.48
1:C:145:LEU:HD12	1:C:147:LEU:HD12	1.96	0.48
1:D:219:LEU:HD11	1:F:237:ILE:HD12	1.94	0.48
1:F:113:LYS:HD2	1:F:195:TYR:CE2	2.48	0.48
1:B:73:ASP:O	1:B:77:PHE:N	2.34	0.48
1:E:133:ASP:OD1	1:E:133:ASP:C	2.56	0.48
1:E:246:GLU:HG2	1:F:209:PRO:HB3	1.96	0.48
1:F:226:GLN:NE2	1:F:226:GLN:H	2.12	0.48
1:F:133:ASP:C	1:F:133:ASP:OD1	2.56	0.47
1:B:12:HIS:CG	1:B:28:ARG:HG3	2.49	0.47
1:F:210:LEU:O	1:F:210:LEU:HG	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:104:LEU:HD23	1:E:108:LEU:HB2	1.97	0.47
1:A:209:PRO:HB3	1:C:246:GLU:HG2	1.96	0.47
1:F:202:ALA:O	1:F:206:THR:HG23	2.14	0.47
1:C:98:LEU:HD13	1:C:151:GLY:HA2	1.97	0.47
1:D:98:LEU:HD13	1:D:151:GLY:HA2	1.96	0.47
1:D:238:PHE:CE2	1:D:242:VAL:HG21	2.50	0.47
1:B:113:LYS:HE2	4:B:339:HOH:O	2.14	0.47
1:F:93:PRO:HB2	1:F:94:PRO:HD3	1.95	0.47
1:C:104:LEU:HD23	1:C:108:LEU:HB2	1.96	0.47
1:E:193:ASP:OD2	1:E:196:ALA:CB	2.63	0.47
1:F:128:ASP:O	1:F:129:LEU:HD23	2.15	0.47
1:F:38:GLU:HG2	4:F:388:HOH:O	2.15	0.46
1:B:74:MET:HA	1:B:77:PHE:CB	2.45	0.46
1:C:10:HIS:HA	1:C:11:PRO:HD3	1.81	0.46
1:D:137:LEU:HD11	1:D:175:LYS:HG2	1.96	0.46
1:E:66:HIS:CD2	4:E:304:HOH:O	2.53	0.46
1:E:155:GLN:OE1	1:E:226:GLN:NE2	2.49	0.46
1:D:57:ARG:HB2	1:D:206:THR:HG22	1.98	0.46
1:A:98:LEU:HD13	1:A:151:GLY:HA2	1.99	0.45
1:C:9:LEU:CD2	1:C:9:LEU:C	2.82	0.45
1:C:202:ALA:O	1:C:206:THR:HG23	2.16	0.45
1:B:73:ASP:HB3	1:B:76:ASP:CB	2.42	0.45
1:A:237:ILE:HD12	1:B:219:LEU:HD21	1.98	0.45
1:C:146:GLY:O	1:C:241:ARG:HD3	2.16	0.45
1:C:226:GLN:N	1:C:226:GLN:CD	2.76	0.44
1:D:148:SER:HB2	1:D:149:PRO:CD	2.48	0.44
1:B:172:THR:OG1	1:B:174:LYS:HD3	2.17	0.44
1:C:203:GLN:NE2	4:C:289:HOH:O	2.40	0.44
1:A:212:SER:OG	1:C:146:GLY:HA2	2.18	0.44
1:A:57:ARG:NH2	4:A:278:HOH:O	2.51	0.44
1:F:199:GLN:O	1:F:203:GLN:HG3	2.18	0.44
1:D:215:GLN:NE2	1:F:237:ILE:HD13	2.33	0.43
1:E:148:SER:HB2	1:E:149:PRO:CD	2.48	0.43
1:E:134:ASN:OD1	1:E:190:ILE:HG21	2.19	0.43
1:B:199:GLN:NE2	1:B:203:GLN:HG3	2.33	0.43
1:C:25:ALA:CB	1:C:62:ARG:HD2	2.49	0.43
1:F:25:ALA:HB1	1:F:64:ALA:HA	1.99	0.43
1:A:98:LEU:HD13	1:A:151:GLY:CA	2.49	0.43
1:D:210:LEU:O	1:D:210:LEU:HG	2.18	0.42
1:D:199:GLN:O	1:D:203:GLN:HG3	2.19	0.42
1:A:74:MET:HA	1:A:74:MET:HE2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:116:ALA:O	1:F:138:PHE:HA	2.19	0.42
1:F:119:ILE:O	1:F:123:ILE:HG22	2.19	0.42
1:A:104:LEU:HD23	1:A:108:LEU:HB2	2.01	0.42
1:D:148:SER:HB2	1:D:149:PRO:HD2	2.01	0.42
1:C:9:LEU:C	1:C:10:HIS:CG	2.97	0.42
1:C:232:ASP:O	1:C:236:GLU:HG2	2.21	0.41
1:D:199:GLN:NE2	1:D:203:GLN:CG	2.83	0.41
1:A:99:LYS:NZ	2:A:3:SO4:O3	2.49	0.41
1:A:148:SER:HB2	1:A:149:PRO:CD	2.50	0.41
1:F:28:ARG:O	1:F:28:ARG:CG	2.68	0.41
1:F:148:SER:HB2	1:F:149:PRO:HD2	2.02	0.41
1:B:53:ASN:OD1	1:B:53:ASN:C	2.62	0.41
1:C:152:GLY:N	1:C:234:GLU:OE1	2.52	0.41
1:B:239:MET:HE2	1:B:239:MET:CA	2.24	0.41
1:B:239:MET:HE2	1:B:242:VAL:HB	2.02	0.41
1:C:242:VAL:O	1:C:242:VAL:CG1	2.65	0.41
1:F:12:HIS:HA	1:F:27:ASN:O	2.20	0.41
1:B:148:SER:HB2	1:B:149:PRO:CD	2.51	0.41
1:C:25:ALA:HB2	1:C:62:ARG:HD2	2.03	0.41
1:E:44:ALA:HB2	1:E:97:LEU:HA	2.02	0.41
1:F:25:ALA:HA	1:F:62:ARG:O	2.20	0.41
1:B:28:ARG:N	1:B:29:PRO:CD	2.84	0.40
1:B:104:LEU:HD23	1:B:108:LEU:HB2	2.03	0.40
1:A:44:ALA:HB3	1:A:45:LYS:HZ3	1.86	0.40
1:A:189:GLU:HG2	1:A:191:VAL:HG13	2.02	0.40
1:B:199:GLN:NE2	1:B:203:GLN:CG	2.84	0.40
1:F:165:LYS:HE2	1:F:165:LYS:HB2	1.87	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)
1:E:192:GLU:OE2	4:C:295:HOH:O[1_545]	1.97	0.23
1:E:240:GLN:NE2	4:F:275:HOH:O[2_656]	2.12	0.08

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	247/266 (93%)	240 (97%)	7 (3%)	0	100	100
1	B	228/266 (86%)	218 (96%)	9 (4%)	1 (0%)	30	27
1	C	223/266 (84%)	215 (96%)	7 (3%)	1 (0%)	30	27
1	D	221/266 (83%)	213 (96%)	8 (4%)	0	100	100
1	E	230/266 (86%)	224 (97%)	5 (2%)	1 (0%)	30	27
1	F	211/266 (79%)	200 (95%)	9 (4%)	2 (1%)	14	9
All	All	1360/1596 (85%)	1310 (96%)	45 (3%)	5 (0%)	30	27

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	32	LYS
1	E	37	GLY
1	F	37	GLY
1	B	37	GLY
1	C	37	GLY

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	192/212 (91%)	187 (97%)	5 (3%)	40	44
1	B	176/212 (83%)	170 (97%)	6 (3%)	32	33
1	C	176/212 (83%)	170 (97%)	6 (3%)	32	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	172/212 (81%)	165 (96%)	7 (4%)	27	26
1	E	179/212 (84%)	176 (98%)	3 (2%)	53	60
1	F	163/212 (77%)	159 (98%)	4 (2%)	42	45
All	All	1058/1272 (83%)	1027 (97%)	31 (3%)	37	40

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	MET
1	A	119	ILE
1	A	150	GLU
1	A	210	LEU
1	A	241	ARG
1	B	16	ASN
1	B	74	MET
1	B	78	MET
1	B	137	LEU
1	B	239	MET
1	B	243	GLN
1	C	62	ARG
1	C	74	MET
1	C	236	GLU
1	C	241	ARG
1	C	242	VAL
1	C	243	GLN
1	D	65	GLU
1	D	74	MET
1	D	75	LYS
1	D	119	ILE
1	D	134	ASN
1	D	137	LEU
1	D	210	LEU
1	E	74	MET
1	E	247	MET
1	E	248	LEU
1	F	16	ASN
1	F	32	LYS
1	F	57	ARG
1	F	174	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	14	ASN
1	A	66	HIS
1	A	233	HIS
1	B	14	ASN
1	B	16	ASN
1	B	27	ASN
1	B	66	HIS
1	B	139	GLN
1	B	199	GLN
1	B	203	GLN
1	B	215	GLN
1	B	222	HIS
1	C	12	HIS
1	C	14	ASN
1	C	183	GLN
1	C	199	GLN
1	C	203	GLN
1	C	222	HIS
1	C	243	GLN
1	D	16	ASN
1	D	134	ASN
1	D	199	GLN
1	D	203	GLN
1	D	222	HIS
1	D	226	GLN
1	D	233	HIS
1	E	155	GLN
1	E	199	GLN
1	E	203	GLN
1	E	226	GLN
1	F	12	HIS
1	F	183	GLN
1	F	203	GLN
1	F	215	GLN
1	F	233	HIS

5.3.3 RNA ⓘ

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](#)

5 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	E	2	-	4,4,4	0.43	0	6,6,6	0.36	0
3	GOL	A	1	-	5,5,5	0.24	0	5,5,5	0.76	0
2	SO4	C	4	-	4,4,4	0.33	0	6,6,6	0.21	0
2	SO4	A	3	-	4,4,4	0.27	0	6,6,6	0.37	0
2	SO4	E	1	-	4,4,4	0.44	0	6,6,6	0.34	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
3	GOL	A	1	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1	GOL	C1-C2-C3-O3
3	A	1	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3	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	248/266 (93%)	-0.30	3 (1%) 76 76	12, 22, 33, 42	1 (0%)
1	B	232/266 (87%)	0.36	19 (8%) 17 16	19, 32, 52, 61	0
1	C	227/266 (85%)	0.17	8 (3%) 47 46	17, 29, 44, 56	0
1	D	225/266 (84%)	0.26	9 (4%) 42 41	23, 33, 44, 59	0
1	E	234/266 (87%)	0.41	12 (5%) 33 32	22, 35, 51, 57	0
1	F	215/266 (80%)	0.59	13 (6%) 27 26	23, 38, 52, 58	0
All	All	1381/1596 (86%)	0.24	64 (4%) 37 36	12, 31, 49, 61	1 (0%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	250	ALA	5.8
1	A	8	SER	5.7
1	D	77	PHE	4.7
1	B	74	MET	4.2
1	E	249	GLU	3.6
1	E	64	ALA	3.4
1	B	236	GLU	3.4
1	F	31	ALA	3.3
1	B	42	TRP	3.2
1	B	244	SER	3.2
1	D	30	GLU	3.2
1	B	248	LEU	3.1
1	B	9	LEU	3.1
1	D	242	VAL	3.1
1	E	82	GLN	3.0
1	E	248	LEU	3.0
1	E	42	TRP	3.0
1	F	42	TRP	3.0
1	E	240	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	16	ASN	2.8
1	C	42	TRP	2.8
1	C	243	GLN	2.8
1	B	65	GLU	2.7
1	D	87	GLY	2.7
1	E	20	GLY	2.7
1	B	78	MET	2.7
1	B	64	ALA	2.6
1	F	240	GLN	2.5
1	F	38	GLU	2.5
1	C	15	ALA	2.5
1	F	135	THR	2.4
1	F	64	ALA	2.4
1	B	77	PHE	2.4
1	A	14	ASN	2.4
1	B	16	ASN	2.4
1	D	134	ASN	2.4
1	B	243	GLN	2.4
1	E	81	VAL	2.4
1	C	240	GLN	2.4
1	B	76	ASP	2.4
1	F	30	GLU	2.2
1	F	203	GLN	2.2
1	C	207	ALA	2.2
1	E	134	ASN	2.2
1	B	88	PRO	2.2
1	C	88	PRO	2.2
1	F	73	ASP	2.2
1	B	11	PRO	2.1
1	F	66	HIS	2.1
1	B	247	MET	2.1
1	A	76	ASP	2.1
1	E	65	GLU	2.1
1	C	225	ASP	2.1
1	C	53	ASN	2.1
1	D	241	ARG	2.1
1	E	242	VAL	2.1
1	B	249	GLU	2.0
1	F	63	GLY	2.0
1	F	236	GLU	2.0
1	D	16	ASN	2.0
1	B	17	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	203	GLN	2.0
1	D	57	ARG	2.0
1	B	37	GLY	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	SO4	E	2	5/5	0.69	0.17	53,56,58,60	0
2	SO4	C	4	5/5	0.83	0.11	66,66,67,68	0
2	SO4	A	3	5/5	0.88	0.18	58,58,61,61	0
3	GOL	A	1	6/6	0.90	0.10	36,39,45,51	0
2	SO4	E	1	5/5	0.95	0.14	47,49,51,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.