Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:08 PM GMT

PDB ID	:	1WKB
Title	:	Crystal Structure of Leucyl-tRNA Synthetase from the Archaeon Pyrococcus horikoshii Reveals a Novel Editing Domain Orientation
Authors	:	Fukunaga, R.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2004-05-30
Resolution	:	2.05 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

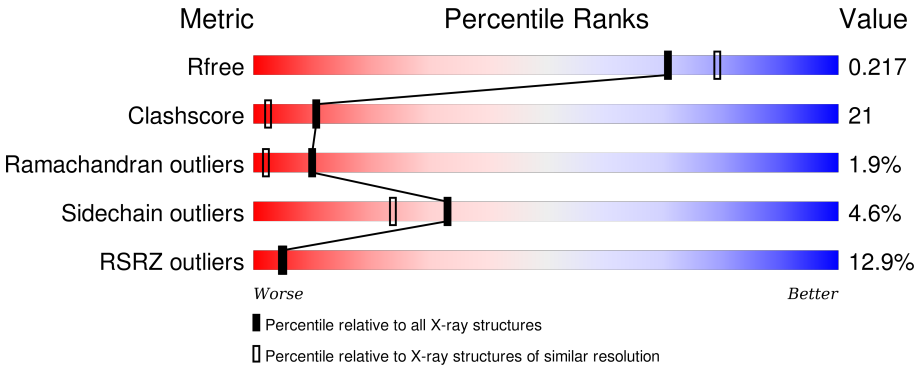
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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}	91344	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	810	13% 66% 27%

2 Entry composition

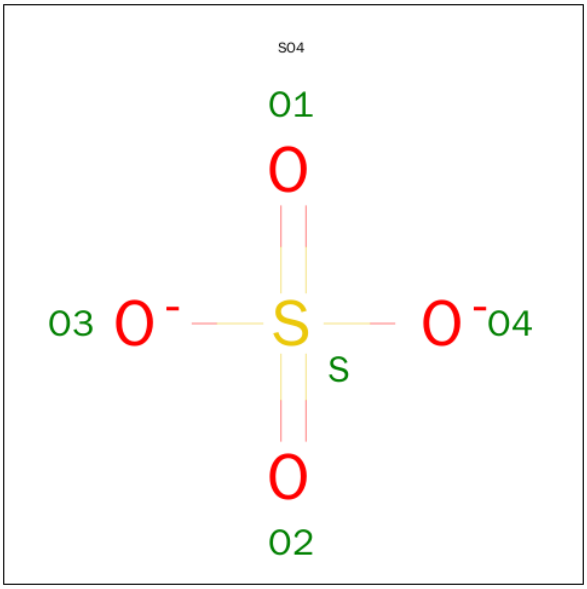
There are 3 unique types of molecules in this entry. The entry contains 7475 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Leucyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	791	Total	C	N	O	S	0	0	0
			6610	4299	1109	1183	19			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

- Molecule 3 is water.

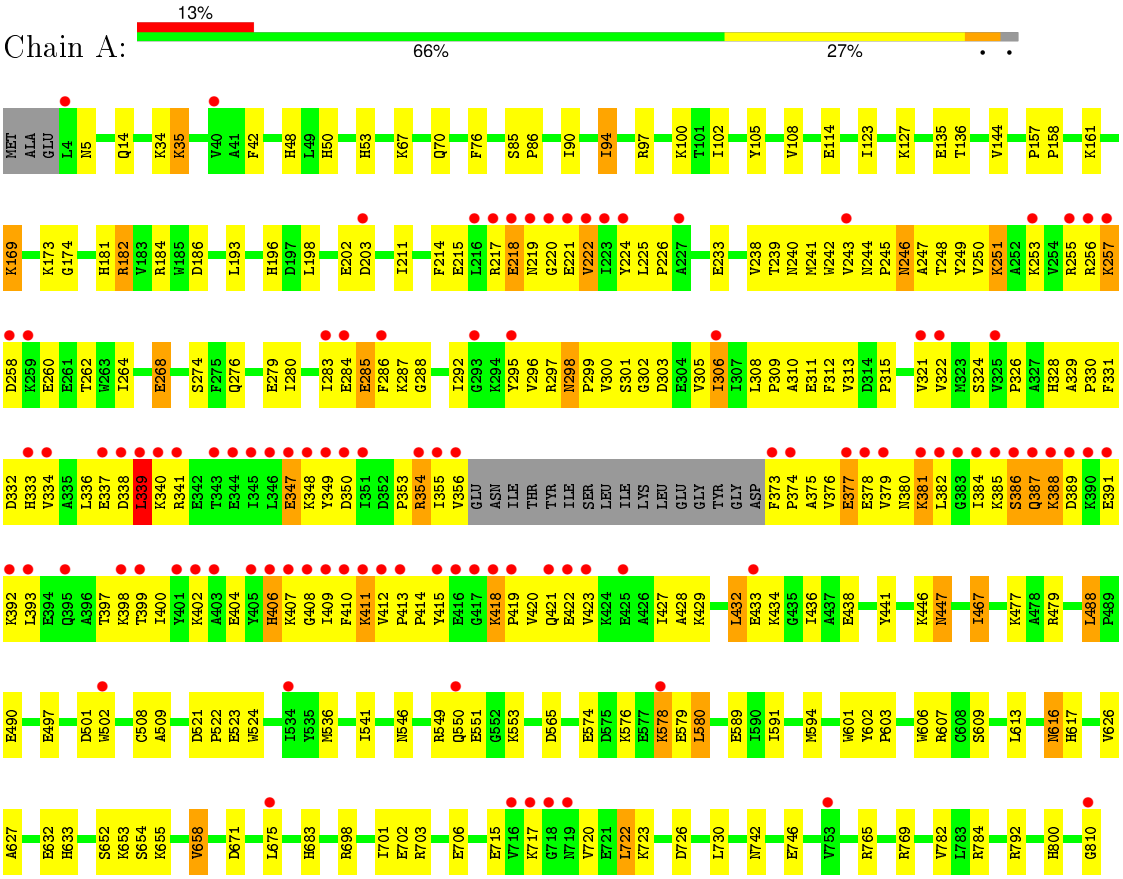
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	825	Total O 825 825	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Leucyl-tRNA synthetase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	186.20Å 186.20Å 91.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.96 – 2.05 28.96 – 2.05	Depositor EDS
% Data completeness (in resolution range)	98.8 (28.96-2.05) 98.9 (28.96-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 2.04Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.180 , 0.218 0.180 , 0.217	Depositor DCC
R_{free} test set	3752 reflections (5.12%)	DCC
Wilson B-factor (Å^2)	33.0	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 71.8	EDS
Estimated twinning fraction	0.014 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 73341 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7475	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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

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	0.55	0/6792	0.69	2/9181 (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	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	251	LYS	N-CA-C	-5.34	96.58	111.00
1	A	467	ILE	N-CA-C	-5.28	96.74	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	TYR	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6610	0	6586	280	0
2	A	40	0	0	3	0
3	A	825	0	0	33	0
All	All	7475	0	6586	280	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 (280) 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:412:VAL:HG12	1:A:414:PRO:HD2	1.36	1.06
1:A:233:GLU:HA	1:A:427:ILE:HD12	1.40	1.00
1:A:546:ASN:O	1:A:550:GLN:HG2	1.67	0.94
1:A:616:ASN:HD22	1:A:617:HIS:H	1.12	0.94
1:A:298:ASN:HD22	1:A:300:VAL:H	1.13	0.94
1:A:50:HIS:H	1:A:53:HIS:HD2	1.13	0.92
1:A:347:GLU:HG3	1:A:348:LYS:HD2	1.48	0.91
1:A:114:GLU:HG3	3:A:1177:HOH:O	1.72	0.90
1:A:447:ASN:HD22	1:A:447:ASN:H	1.24	0.85
1:A:274:SER:HA	1:A:280:ILE:HD13	1.61	0.82
1:A:354:ARG:HH21	1:A:356:VAL:HB	1.43	0.82
1:A:388:LYS:HD2	1:A:388:LYS:H	1.45	0.82
1:A:246:ASN:HD22	1:A:246:ASN:N	1.77	0.82
1:A:298:ASN:ND2	1:A:300:VAL:H	1.77	0.81
1:A:301:SER:O	1:A:303:ASP:N	2.14	0.80
1:A:429:LYS:O	1:A:433:GLU:HG2	1.84	0.78
1:A:50:HIS:H	1:A:53:HIS:CD2	2.02	0.78
1:A:378:GLU:HA	1:A:381:LYS:HZ2	1.49	0.77
1:A:276:GLN:HE22	1:A:441:TYR:H	1.29	0.77
1:A:306:ILE:N	1:A:306:ILE:HD13	2.00	0.76
1:A:404:GLU:O	1:A:420:VAL:HG11	1.86	0.76
1:A:214:PHE:HB3	1:A:296:VAL:HG21	1.68	0.74
1:A:607:ARG:HE	1:A:617:HIS:HE1	1.36	0.73
1:A:248:THR:CG2	1:A:285:GLU:HG3	2.18	0.73
1:A:413:PRO:HB2	1:A:414:PRO:HD3	1.70	0.72
1:A:295:TYR:CZ	1:A:306:ILE:HG23	2.25	0.72
1:A:354:ARG:HG2	1:A:375:ALA:HB1	1.71	0.71
1:A:671:ASP:OD1	1:A:800:HIS:HD2	1.73	0.71
1:A:284:GLU:HB3	1:A:286:PHE:CZ	2.25	0.71
1:A:378:GLU:HA	1:A:381:LYS:NZ	2.04	0.71
1:A:214:PHE:HB3	1:A:296:VAL:CG2	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:616:ASN:ND2	1:A:617:HIS:H	1.88	0.70
1:A:574:GLU:O	1:A:578:LYS:HE3	1.90	0.70
1:A:238:VAL:HA	1:A:324:SER:O	1.92	0.70
1:A:233:GLU:HA	1:A:427:ILE:CD1	2.21	0.69
1:A:306:ILE:HD13	1:A:306:ILE:H	1.57	0.69
1:A:222:VAL:O	1:A:262:THR:HB	1.93	0.68
1:A:248:THR:HG21	1:A:285:GLU:HG3	1.76	0.68
1:A:182:ARG:H	1:A:182:ARG:HD3	1.59	0.68
1:A:310:ALA:O	1:A:313:VAL:HG12	1.93	0.68
1:A:326:PRO:HG2	1:A:336:LEU:HD11	1.76	0.67
1:A:784:ARG:HH22	1:A:810:GLY:H	1.43	0.67
1:A:354:ARG:C	1:A:354:ARG:HD3	2.15	0.67
1:A:243:VAL:HG13	1:A:249:TYR:CZ	2.30	0.66
1:A:633:HIS:HE1	3:A:967:HOH:O	1.80	0.65
1:A:355:ILE:HG21	1:A:410:PHE:CE1	2.31	0.65
1:A:215:GLU:C	1:A:296:VAL:HG23	2.15	0.65
1:A:769:ARG:HD3	3:A:1066:HOH:O	1.96	0.65
1:A:246:ASN:N	1:A:246:ASN:ND2	2.44	0.65
1:A:253:LYS:CE	1:A:255:ARG:HH22	2.10	0.64
1:A:330:PRO:CG	1:A:400:ILE:HD12	2.28	0.64
1:A:330:PRO:HG3	1:A:400:ILE:HD12	1.78	0.64
1:A:391:GLU:C	1:A:393:LEU:H	2.01	0.64
1:A:378:GLU:HG2	1:A:381:LYS:HD2	1.79	0.64
1:A:490:GLU:OE2	3:A:1677:HOH:O	2.13	0.64
1:A:298:ASN:C	1:A:298:ASN:HD22	2.00	0.64
1:A:242:TRP:HB2	1:A:322:VAL:HB	1.79	0.64
1:A:298:ASN:HD21	1:A:300:VAL:HB	1.63	0.64
1:A:67:LYS:NZ	1:A:70:GLN:HE22	1.96	0.64
1:A:310:ALA:HB1	1:A:312:PHE:CD1	2.33	0.63
1:A:423:VAL:O	1:A:427:ILE:HG13	1.99	0.63
1:A:251:LYS:HB2	1:A:286:PHE:HE2	1.63	0.63
1:A:549:ARG:HD3	3:A:1412:HOH:O	1.98	0.63
1:A:412:VAL:CG1	1:A:414:PRO:HD2	2.23	0.63
1:A:410:PHE:CD2	1:A:415:TYR:HB2	2.35	0.62
1:A:393:LEU:HD13	1:A:393:LEU:O	1.99	0.62
1:A:14:GLN:HE21	1:A:800:HIS:CE1	2.18	0.62
1:A:347:GLU:CG	1:A:348:LYS:H	2.12	0.61
1:A:251:LYS:HB2	1:A:286:PHE:CE2	2.36	0.61
1:A:355:ILE:HG22	1:A:355:ILE:O	2.01	0.61
1:A:333:HIS:ND1	1:A:381:LYS:HG3	2.16	0.61
1:A:354:ARG:O	1:A:354:ARG:HD3	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ARG:HD3	1:A:218:GLU:N	2.17	0.60
1:A:50:HIS:N	1:A:53:HIS:HD2	1.94	0.60
1:A:35:LYS:HE2	1:A:601:TRP:O	2.02	0.59
1:A:374:PRO:O	1:A:377:GLU:HG3	2.01	0.59
1:A:100:LYS:NZ	1:A:654:SER:HB3	2.17	0.59
1:A:337:GLU:O	1:A:388:LYS:HE3	2.03	0.59
1:A:376:VAL:O	1:A:378:GLU:N	2.37	0.58
1:A:723:LYS:HE3	3:A:1547:HOH:O	2.04	0.58
1:A:384:ILE:O	1:A:385:LYS:HB2	2.02	0.58
1:A:386:SER:O	1:A:387:GLN:HB2	2.04	0.57
1:A:330:PRO:HB2	1:A:397:THR:HG22	1.87	0.57
1:A:240:ASN:HB2	1:A:308:LEU:HD13	1.85	0.57
1:A:334:VAL:HG23	1:A:388:LYS:HA	1.86	0.57
1:A:412:VAL:HG13	1:A:413:PRO:HD2	1.86	0.57
1:A:292:ILE:HG13	1:A:309:PRO:HG3	1.86	0.57
1:A:241:MET:CE	1:A:305:VAL:HG21	2.35	0.57
1:A:381:LYS:HZ1	1:A:400:ILE:HD11	1.69	0.57
1:A:135:GLU:HB2	3:A:1251:HOH:O	2.04	0.57
1:A:388:LYS:N	1:A:388:LYS:HD2	2.17	0.56
1:A:765:ARG:CZ	3:A:1366:HOH:O	2.53	0.56
1:A:310:ALA:HB1	1:A:312:PHE:HD1	1.71	0.56
1:A:218:GLU:O	1:A:220:GLY:N	2.38	0.56
1:A:479:ARG:NH2	1:A:501:ASP:OD1	2.36	0.56
1:A:633:HIS:HD2	3:A:1347:HOH:O	1.89	0.56
1:A:90:ILE:O	1:A:94:ILE:HG23	2.05	0.56
1:A:398:LYS:HG3	1:A:399:THR:N	2.20	0.56
1:A:347:GLU:C	1:A:349:TYR:H	2.08	0.56
1:A:420:VAL:HG13	1:A:421:GLN:N	2.21	0.56
1:A:347:GLU:CG	1:A:348:LYS:N	2.69	0.56
1:A:347:GLU:HG3	1:A:348:LYS:N	2.20	0.56
1:A:324:SER:OG	1:A:332:ASP:HB3	2.05	0.56
1:A:274:SER:CA	1:A:280:ILE:HD13	2.32	0.56
1:A:218:GLU:C	1:A:220:GLY:H	2.09	0.56
1:A:410:PHE:HB3	1:A:415:TYR:O	2.06	0.55
1:A:169:LYS:HE3	1:A:565:ASP:OD1	2.06	0.55
1:A:244:ASN:HD22	1:A:247:ALA:N	2.05	0.55
1:A:298:ASN:ND2	1:A:301:SER:H	2.05	0.55
1:A:400:ILE:O	1:A:404:GLU:HG3	2.07	0.55
1:A:769:ARG:HD3	3:A:1549:HOH:O	2.07	0.54
1:A:477:LYS:HG2	1:A:626:VAL:HB	1.89	0.54
1:A:410:PHE:CE2	1:A:412:VAL:HB	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:ARG:NH2	1:A:356:VAL:HB	2.19	0.54
1:A:214:PHE:HA	1:A:299:PRO:HD3	1.88	0.54
1:A:589:GLU:CD	1:A:589:GLU:H	2.12	0.54
1:A:356:VAL:HG12	1:A:356:VAL:O	2.08	0.53
1:A:574:GLU:HG2	1:A:578:LYS:CE	2.38	0.53
1:A:253:LYS:HE2	1:A:255:ARG:HH22	1.72	0.53
1:A:244:ASN:HB2	1:A:313:VAL:HG13	1.90	0.53
1:A:391:GLU:C	1:A:393:LEU:N	2.59	0.53
1:A:347:GLU:HG3	1:A:348:LYS:H	1.70	0.53
1:A:217:ARG:NE	1:A:220:GLY:O	2.40	0.53
1:A:225:LEU:HG	1:A:321:VAL:HG11	1.91	0.53
1:A:792:ARG:HB2	3:A:1428:HOH:O	2.09	0.53
1:A:447:ASN:N	1:A:447:ASN:HD22	1.99	0.53
1:A:330:PRO:HG3	1:A:381:LYS:HE3	1.89	0.53
1:A:617:HIS:HD2	3:A:915:HOH:O	1.92	0.53
1:A:467:ILE:HG13	1:A:508:CYS:HB3	1.91	0.53
1:A:251:LYS:CB	1:A:286:PHE:HE2	2.21	0.53
1:A:241:MET:HE2	1:A:305:VAL:HG21	1.90	0.52
1:A:295:TYR:CE1	1:A:306:ILE:HG23	2.44	0.52
1:A:268:GLU:HG3	1:A:315:PRO:O	2.09	0.52
1:A:347:GLU:OE2	1:A:347:GLU:HA	2.10	0.52
1:A:196:HIS:HD2	2:A:901:SO4:O3	1.92	0.52
1:A:328:HIS:CE1	1:A:355:ILE:H	2.28	0.52
1:A:35:LYS:NZ	1:A:603:PRO:O	2.40	0.52
1:A:97:ARG:HA	1:A:102:ILE:HD11	1.92	0.52
1:A:14:GLN:HE21	1:A:800:HIS:HE1	1.58	0.52
1:A:765:ARG:O	1:A:769:ARG:HG3	2.10	0.52
1:A:215:GLU:O	1:A:296:VAL:HG23	2.10	0.51
1:A:378:GLU:HA	1:A:381:LYS:CD	2.41	0.51
1:A:703:ARG:HG2	3:A:1665:HOH:O	2.10	0.51
1:A:702:GLU:O	1:A:706:GLU:HG3	2.10	0.51
1:A:373:PHE:N	1:A:374:PRO:CD	2.74	0.51
1:A:502:TRP:HB3	3:A:1672:HOH:O	2.10	0.51
1:A:523:GLU:HG3	3:A:1236:HOH:O	2.09	0.51
1:A:283:ILE:O	1:A:284:GLU:HB2	2.10	0.51
1:A:308:LEU:N	1:A:308:LEU:HD12	2.26	0.51
1:A:347:GLU:CD	1:A:348:LYS:H	2.13	0.50
1:A:108:VAL:HG13	1:A:658:VAL:HG22	1.93	0.50
1:A:550:GLN:HG3	3:A:1708:HOH:O	2.11	0.50
1:A:196:HIS:HE1	3:A:1559:HOH:O	1.94	0.50
1:A:376:VAL:O	1:A:378:GLU:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:607:ARG:HH21	1:A:617:HIS:CE1	2.30	0.50
1:A:233:GLU:CA	1:A:427:ILE:HD12	2.28	0.50
1:A:238:VAL:HG22	3:A:1145:HOH:O	2.12	0.50
1:A:244:ASN:HD22	1:A:247:ALA:H	1.60	0.49
1:A:123:ILE:HG22	1:A:127:LYS:HE2	1.93	0.49
1:A:157:PRO:HB2	1:A:158:PRO:HD3	1.93	0.49
1:A:765:ARG:NH2	3:A:1162:HOH:O	2.35	0.49
1:A:387:GLN:O	1:A:389:ASP:N	2.45	0.49
1:A:217:ARG:HA	1:A:217:ARG:NE	2.27	0.49
1:A:301:SER:C	1:A:303:ASP:H	2.13	0.49
1:A:551:GLU:HB3	1:A:553:LYS:HG3	1.95	0.49
1:A:576:LYS:HA	1:A:579:GLU:HG2	1.95	0.49
1:A:211:ILE:HG12	1:A:438:GLU:O	2.13	0.48
1:A:580:LEU:HB3	1:A:591:ILE:HD13	1.95	0.48
1:A:240:ASN:C	1:A:241:MET:HE2	2.34	0.48
1:A:211:ILE:HG13	1:A:211:ILE:O	2.14	0.48
1:A:250:VAL:O	1:A:264:ILE:HA	2.12	0.48
1:A:410:PHE:HB2	1:A:423:VAL:HG21	1.96	0.48
1:A:245:PRO:HG2	1:A:246:ASN:ND2	2.27	0.48
1:A:386:SER:O	1:A:387:GLN:CB	2.61	0.48
1:A:355:ILE:HA	1:A:411:LYS:HB3	1.96	0.48
1:A:334:VAL:HG11	1:A:393:LEU:HD21	1.95	0.48
1:A:378:GLU:HA	1:A:381:LYS:HD2	1.96	0.48
1:A:338:ASP:O	1:A:339:LEU:HB3	2.14	0.47
1:A:447:ASN:ND2	1:A:447:ASN:H	2.04	0.47
1:A:353:PRO:HD3	3:A:1474:HOH:O	2.15	0.47
1:A:380:ASN:C	1:A:382:LEU:H	2.17	0.47
1:A:418:LYS:HD3	1:A:422:GLU:OE2	2.13	0.47
1:A:423:VAL:HG12	1:A:427:ILE:HD11	1.95	0.47
1:A:398:LYS:NZ	1:A:402:LYS:HE3	2.29	0.47
1:A:384:ILE:O	1:A:384:ILE:HG22	2.15	0.47
1:A:683:HIS:HE1	1:A:746:GLU:O	1.98	0.46
1:A:378:GLU:CA	1:A:381:LYS:HZ2	2.25	0.46
1:A:381:LYS:NZ	1:A:400:ILE:HD11	2.30	0.46
1:A:418:LYS:HA	1:A:418:LYS:HE3	1.97	0.46
1:A:67:LYS:HD3	1:A:70:GLN:HE21	1.81	0.46
1:A:135:GLU:HG3	1:A:136:THR:N	2.30	0.46
1:A:497:GLU:HG2	3:A:1414:HOH:O	2.14	0.46
1:A:376:VAL:HG23	1:A:376:VAL:O	2.16	0.46
1:A:245:PRO:HA	1:A:288:GLY:HA3	1.97	0.46
1:A:410:PHE:HD2	1:A:415:TYR:HB2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ASP:HB2	1:A:193:LEU:HD21	1.98	0.46
1:A:341:ARG:HD2	1:A:341:ARG:N	2.31	0.46
1:A:295:TYR:HA	1:A:305:VAL:O	2.16	0.46
1:A:48:HIS:HE1	3:A:1024:HOH:O	1.97	0.46
1:A:239:THR:OG1	1:A:240:ASN:ND2	2.49	0.46
1:A:100:LYS:HZ3	1:A:654:SER:CB	2.28	0.46
1:A:328:HIS:HD2	1:A:404:GLU:OE1	1.99	0.46
1:A:720:VAL:HG23	1:A:722:LEU:HD13	1.98	0.46
1:A:310:ALA:HB1	1:A:312:PHE:CE1	2.52	0.45
1:A:574:GLU:HG2	1:A:578:LYS:HE2	1.99	0.45
1:A:181:HIS:HE1	3:A:1260:HOH:O	2.00	0.45
1:A:330:PRO:HD2	1:A:397:THR:HG22	1.98	0.45
1:A:242:TRP:O	1:A:243:VAL:HG23	2.17	0.45
1:A:521:ASP:N	1:A:522:PRO:HD3	2.32	0.45
1:A:446:LYS:HA	3:A:1052:HOH:O	2.17	0.45
1:A:67:LYS:HZ2	1:A:70:GLN:HE22	1.62	0.45
1:A:742:ASN:ND2	3:A:1015:HOH:O	2.50	0.45
1:A:85:SER:N	1:A:86:PRO:CD	2.80	0.44
1:A:184:ARG:NH2	2:A:906:SO4:O4	2.50	0.44
1:A:279:GLU:C	1:A:280:ILE:HD12	2.37	0.44
1:A:385:LYS:N	1:A:385:LYS:HD2	2.31	0.44
1:A:467:ILE:HG13	1:A:508:CYS:CB	2.48	0.44
1:A:339:LEU:O	1:A:340:LYS:HD3	2.17	0.44
1:A:653:LYS:HE3	1:A:653:LYS:HB3	1.82	0.44
1:A:280:ILE:N	1:A:280:ILE:HD12	2.33	0.44
1:A:306:ILE:CD1	1:A:306:ILE:H	2.17	0.44
1:A:173:LYS:HE2	1:A:627:ALA:O	2.18	0.44
1:A:312:PHE:CE2	1:A:331:PHE:HB3	2.53	0.44
1:A:182:ARG:HD3	1:A:182:ARG:N	2.31	0.44
1:A:268:GLU:HG2	1:A:268:GLU:H	1.32	0.43
1:A:683:HIS:HD2	3:A:1288:HOH:O	2.00	0.43
1:A:549:ARG:NH2	3:A:1271:HOH:O	2.51	0.43
1:A:100:LYS:HZ1	1:A:654:SER:HB3	1.82	0.43
1:A:715:GLU:OE2	1:A:717:LYS:NZ	2.38	0.43
1:A:198:LEU:HB2	1:A:202:GLU:HG3	2.00	0.43
1:A:419:PRO:O	1:A:423:VAL:HG23	2.19	0.43
1:A:287:LYS:HB3	1:A:288:GLY:H	1.66	0.43
1:A:255:ARG:NH2	1:A:260:GLU:HG3	2.34	0.43
1:A:255:ARG:CZ	1:A:260:GLU:HG3	2.49	0.43
1:A:432:LEU:HA	1:A:432:LEU:HD12	1.92	0.43
1:A:723:LYS:HG3	3:A:1439:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:652:SER:OG	1:A:655:LYS:HG3	2.19	0.43
1:A:698:ARG:O	1:A:702:GLU:HG3	2.18	0.43
1:A:488:LEU:HD22	1:A:606:TRP:CH2	2.54	0.43
1:A:420:VAL:CG1	1:A:421:GLN:N	2.82	0.42
1:A:423:VAL:HG12	1:A:427:ILE:CD1	2.49	0.42
1:A:347:GLU:C	1:A:349:TYR:N	2.73	0.42
1:A:34:LYS:NZ	3:A:1143:HOH:O	2.52	0.42
1:A:703:ARG:NH2	3:A:1366:HOH:O	2.45	0.42
1:A:726:ASP:HB3	1:A:782:VAL:HG21	2.00	0.42
1:A:256:ARG:O	1:A:257:LYS:HB2	2.20	0.42
1:A:356:VAL:C	1:A:409:ILE:O	2.58	0.42
1:A:299:PRO:HB2	1:A:436:ILE:HG23	2.00	0.42
1:A:609:SER:HB2	1:A:613:LEU:HD12	2.00	0.42
1:A:298:ASN:C	1:A:298:ASN:ND2	2.72	0.42
1:A:374:PRO:HG3	1:A:379:VAL:CG2	2.50	0.42
1:A:218:GLU:OE2	1:A:218:GLU:O	2.37	0.42
1:A:298:ASN:HB3	1:A:301:SER:O	2.20	0.42
1:A:509:ALA:HB1	1:A:524:TRP:HB3	2.02	0.42
1:A:348:LYS:N	1:A:348:LYS:HD2	2.35	0.42
1:A:521:ASP:OD2	3:A:1236:HOH:O	2.21	0.42
1:A:541:ILE:HB	1:A:594:MET:HE3	2.02	0.42
1:A:428:ALA:O	1:A:432:LEU:HB2	2.20	0.41
1:A:653:LYS:N	2:A:902:SO4:O3	2.53	0.41
1:A:203:ASP:N	1:A:203:ASP:OD1	2.50	0.41
1:A:221:GLU:O	1:A:222:VAL:HG13	2.21	0.41
1:A:174:GLY:HA2	3:A:963:HOH:O	2.21	0.41
1:A:173:LYS:CE	1:A:627:ALA:O	2.68	0.41
1:A:214:PHE:HB3	1:A:296:VAL:HG22	1.99	0.41
1:A:100:LYS:HZ3	1:A:654:SER:HB3	1.84	0.41
1:A:97:ARG:CA	1:A:102:ILE:HD11	2.50	0.41
1:A:374:PRO:HG2	1:A:377:GLU:HA	2.03	0.41
1:A:215:GLU:HB2	1:A:297:ARG:HB3	2.02	0.41
1:A:329:ALA:HB3	1:A:332:ASP:OD2	2.21	0.41
1:A:398:LYS:HZ2	1:A:402:LYS:HE3	1.86	0.41
1:A:157:PRO:O	1:A:161:LYS:HG2	2.20	0.41
1:A:632:GLU:HB3	3:A:1064:HOH:O	2.20	0.41
1:A:224:TYR:O	1:A:226:PRO:HD3	2.20	0.41
1:A:241:MET:HE3	1:A:305:VAL:HG21	2.02	0.41
1:A:76:PHE:O	1:A:144:VAL:HA	2.21	0.41
1:A:675:LEU:HD23	1:A:701:ILE:HD11	2.03	0.41
1:A:331:PHE:CD2	1:A:397:THR:HG21	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:LEU:HD12	1:A:202:GLU:HA	2.03	0.40
1:A:356:VAL:HG22	1:A:377:GLU:OE1	2.21	0.40
1:A:217:ARG:HD3	1:A:218:GLU:H	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	787/810 (97%)	725 (92%)	47 (6%)	15 (2%)	10 2

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	302	GLY
1	A	339	LEU
1	A	377	GLU
1	A	388	LYS
1	A	219	ASN
1	A	347	GLU
1	A	387	GLN
1	A	406	HIS
1	A	408	GLY
1	A	434	LYS
1	A	386	SER
1	A	257	LYS
1	A	350	ASP
1	A	407	LYS
1	A	222	VAL

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	702/718 (98%)	670 (95%)	32 (5%)	33 24

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	35	LYS
1	A	42	PHE
1	A	94	ILE
1	A	169	LYS
1	A	182	ARG
1	A	218	GLU
1	A	246	ASN
1	A	258	ASP
1	A	268	GLU
1	A	285	GLU
1	A	298	ASN
1	A	306	ILE
1	A	311	GLU
1	A	339	LEU
1	A	354	ARG
1	A	381	LYS
1	A	392	LYS
1	A	406	HIS
1	A	411	LYS
1	A	418	LYS
1	A	432	LEU
1	A	447	ASN
1	A	488	LEU
1	A	536	MET
1	A	578	LYS
1	A	580	LEU
1	A	602	TYR
1	A	616	ASN
1	A	658	VAL

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Mol	Chain	Res	Type
1	A	722	LEU
1	A	730	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	26	ASN
1	A	48	HIS
1	A	53	HIS
1	A	70	GLN
1	A	124	ASN
1	A	166	GLN
1	A	181	HIS
1	A	196	HIS
1	A	240	ASN
1	A	244	ASN
1	A	246	ASN
1	A	276	GLN
1	A	298	ASN
1	A	328	HIS
1	A	387	GLN
1	A	421	GLN
1	A	447	ASN
1	A	544	HIS
1	A	616	ASN
1	A	617	HIS
1	A	633	HIS
1	A	683	HIS
1	A	719	ASN
1	A	742	ASN
1	A	800	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

8 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	A	901	-	4,4,4	0.21	0	6,6,6	0.11	0
2	SO4	A	902	-	4,4,4	0.22	0	6,6,6	0.07	0
2	SO4	A	903	-	4,4,4	0.35	0	6,6,6	0.40	0
2	SO4	A	904	-	4,4,4	0.28	0	6,6,6	0.46	0
2	SO4	A	905	-	4,4,4	0.24	0	6,6,6	0.09	0
2	SO4	A	906	-	4,4,4	0.20	0	6,6,6	0.43	0
2	SO4	A	907	-	4,4,4	0.31	0	6,6,6	0.13	0
2	SO4	A	908	-	4,4,4	0.33	0	6,6,6	0.26	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
2	SO4	A	901	-	-	0/0/0/0	0/0/0/0
2	SO4	A	902	-	-	0/0/0/0	0/0/0/0
2	SO4	A	903	-	-	0/0/0/0	0/0/0/0
2	SO4	A	904	-	-	0/0/0/0	0/0/0/0
2	SO4	A	905	-	-	0/0/0/0	0/0/0/0
2	SO4	A	906	-	-	0/0/0/0	0/0/0/0
2	SO4	A	907	-	-	0/0/0/0	0/0/0/0
2	SO4	A	908	-	-	0/0/0/0	0/0/0/0

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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	SO4	1	0
2	A	902	SO4	1	0
2	A	906	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, 95^{th} 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	791/810 (97%)	0.42	102 (12%) 5 5	19, 36, 117, 147	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	222	VAL	9.9
1	A	346	LEU	8.6
1	A	382	LEU	8.5
1	A	384	ILE	8.1
1	A	386	SER	8.0
1	A	351	ILE	7.4
1	A	409	ILE	7.0
1	A	341	ARG	7.0
1	A	385	LYS	6.9
1	A	390	LYS	6.9
1	A	349	TYR	6.8
1	A	810	GLY	6.6
1	A	4	LEU	6.1
1	A	387	GLN	6.1
1	A	347	GLU	6.0
1	A	258	ASP	5.7
1	A	219	ASN	5.7
1	A	286	PHE	5.4
1	A	343	THR	5.4
1	A	338	ASP	5.4
1	A	411	LYS	5.4
1	A	217	ARG	5.4
1	A	410	PHE	5.3
1	A	218	GLU	5.2
1	A	306	ILE	5.2
1	A	399	THR	5.1
1	A	416	GLU	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	502	TRP	5.0
1	A	339	LEU	5.0
1	A	405	TYR	4.9
1	A	417	GLY	4.9
1	A	295	TYR	4.7
1	A	381	LYS	4.7
1	A	221	GLU	4.6
1	A	345	ILE	4.6
1	A	340	LYS	4.6
1	A	406	HIS	4.6
1	A	293	GLY	4.5
1	A	344	GLU	4.5
1	A	412	VAL	4.4
1	A	413	PRO	4.2
1	A	259	LYS	4.2
1	A	379	VAL	4.1
1	A	389	ASP	4.1
1	A	356	VAL	4.1
1	A	220	GLY	4.0
1	A	391	GLU	4.0
1	A	717	LYS	4.0
1	A	322	VAL	4.0
1	A	423	VAL	3.9
1	A	407	LYS	3.8
1	A	421	GLN	3.8
1	A	719	ASN	3.8
1	A	374	PRO	3.7
1	A	348	LYS	3.6
1	A	718	GLY	3.6
1	A	377	GLU	3.5
1	A	350	ASP	3.4
1	A	256	ARG	3.4
1	A	388	LYS	3.4
1	A	392	LYS	3.4
1	A	321	VAL	3.4
1	A	419	PRO	3.3
1	A	401	TYR	3.3
1	A	283	ILE	3.2
1	A	395	GLN	3.2
1	A	716	VAL	3.0
1	A	253	LYS	3.0
1	A	203	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	284	GLU	2.8
1	A	378	GLU	2.8
1	A	418	LYS	2.7
1	A	334	VAL	2.7
1	A	408	GLY	2.7
1	A	403	ALA	2.7
1	A	257	LYS	2.7
1	A	433	GLU	2.7
1	A	355	ILE	2.6
1	A	415	TYR	2.6
1	A	216	LEU	2.6
1	A	398	LYS	2.5
1	A	227	ALA	2.5
1	A	393	LEU	2.5
1	A	675	LEU	2.5
1	A	325	VAL	2.4
1	A	383	GLY	2.3
1	A	40	VAL	2.3
1	A	333	HIS	2.3
1	A	753	VAL	2.2
1	A	223	ILE	2.2
1	A	425	GLU	2.2
1	A	243	VAL	2.2
1	A	255	ARG	2.1
1	A	402	LYS	2.1
1	A	354	ARG	2.1
1	A	337	GLU	2.1
1	A	534	ILE	2.1
1	A	224	TYR	2.1
1	A	550	GLN	2.1
1	A	422	GLU	2.0
1	A	373	PHE	2.0
1	A	578	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	SO4	A	902	5/5	0.95	0.18	1.37	81,85,86,89	0
2	SO4	A	903	5/5	0.96	0.17	0.10	53,55,61,68	0
2	SO4	A	901	5/5	0.99	0.10	-0.02	42,46,51,53	0
2	SO4	A	908	5/5	0.97	0.08	-1.23	46,54,56,60	0
2	SO4	A	906	5/5	0.98	0.07	-1.36	45,49,52,54	0
2	SO4	A	907	5/5	0.98	0.10	-1.46	53,59,65,69	0
2	SO4	A	904	5/5	0.97	0.15	-	44,46,54,61	0
2	SO4	A	905	5/5	0.95	0.09	-	75,77,82,84	0

6.5 Other polymers

There are no such residues in this entry.