Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:58 PM GMT

PDB ID	:	3VK2
Title	:	Crystal Structure of L-Methionine gamma-Lyase from Pseudomonas putida C116H Mutant.
Authors	:	Fukumoto, M.; Kudou, D.; Murano, S.; Shiba, T.; Sato, D.; Tamura, T.; Harada, S.; Inagaki, K.
Deposited on	:	2011-11-07
Resolution	:	2.30 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:

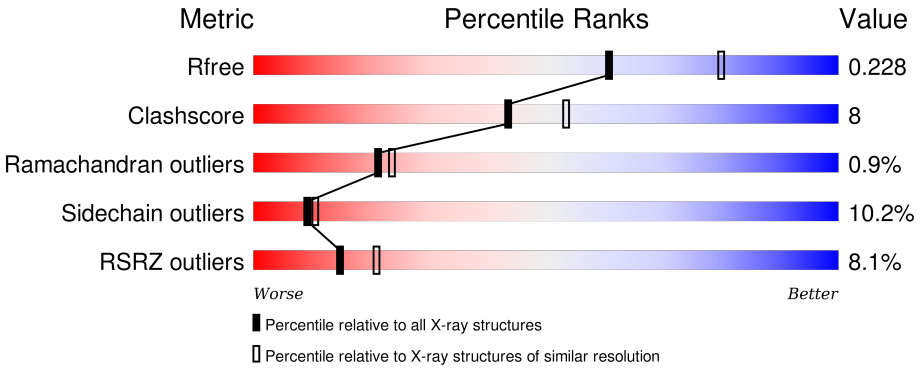
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	398	8% 81% 15%
1	B	398	9% 80% 16%
1	C	398	7% 80% 16%
1	D	398	8% 77% 18%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	C	501	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12350 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.

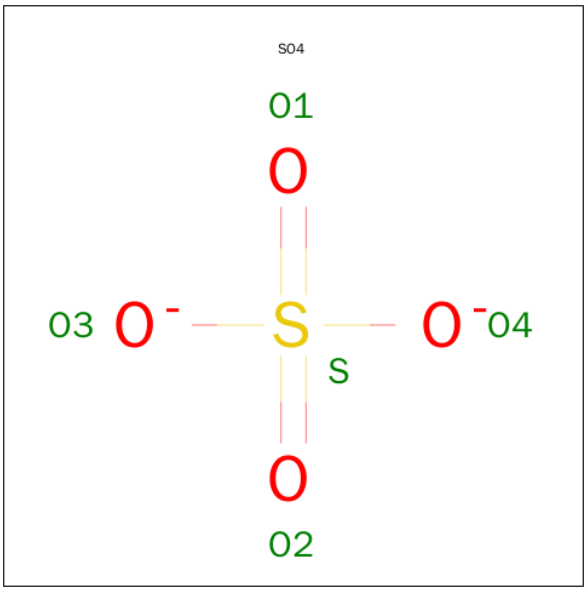
- Molecule 1 is a protein called Methionine gamma-lyase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	393	Total	C	N	O	P	S	0	0	0
			2979	1880	527	555	1	16			
1	B	396	Total	C	N	O	P	S	0	0	0
			2997	1889	531	560	1	16			
1	C	392	Total	C	N	O	P	S	0	0	0
			2970	1874	525	554	1	16			
1	D	393	Total	C	N	O	P	S	0	0	0
			2979	1880	527	555	1	16			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	116	HIS	CYS	ENGINEERED MUTATION	UNP P13254
B	116	HIS	CYS	ENGINEERED MUTATION	UNP P13254
C	116	HIS	CYS	ENGINEERED MUTATION	UNP P13254
D	116	HIS	CYS	ENGINEERED MUTATION	UNP P13254

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



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

- Molecule 3 is water.

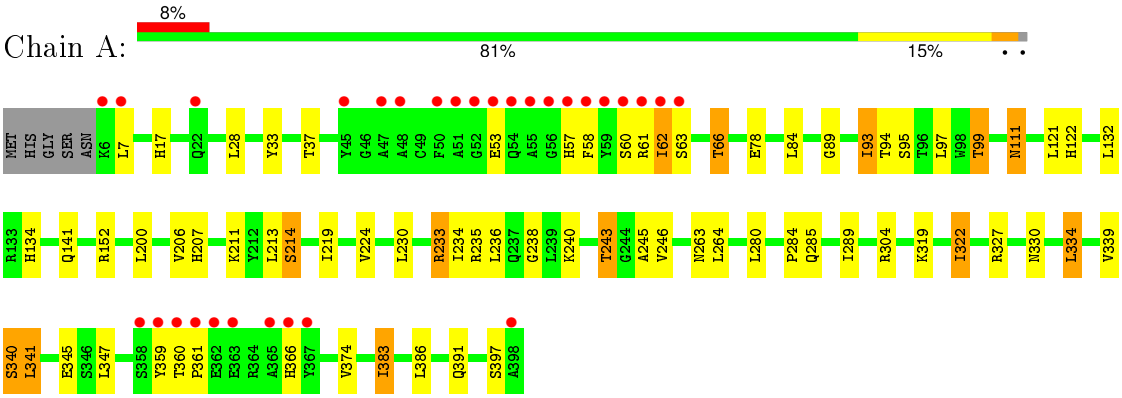
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	99	Total O 99 99	0	0
3	B	115	Total O 115 115	0	0
3	C	110	Total O 110 110	0	0
3	D	81	Total O 81 81	0	0

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.

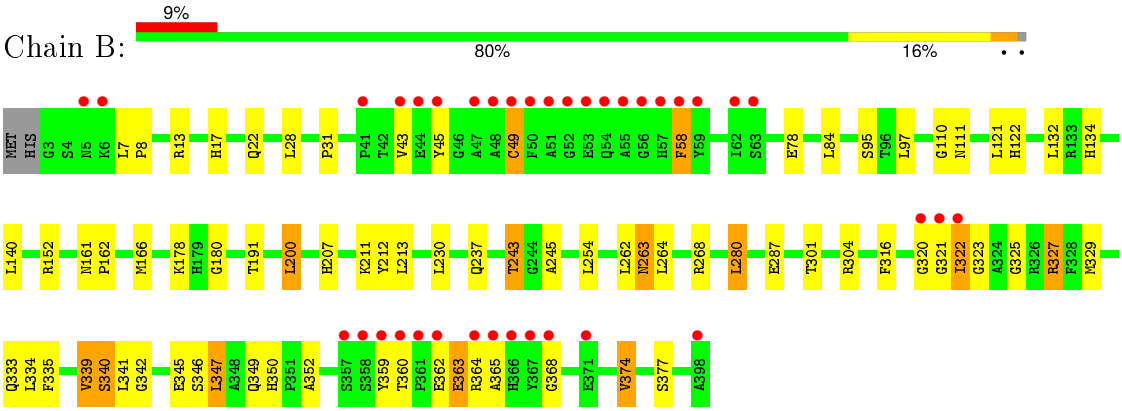
- Molecule 1: Methionine gamma-lyase

Chain A:



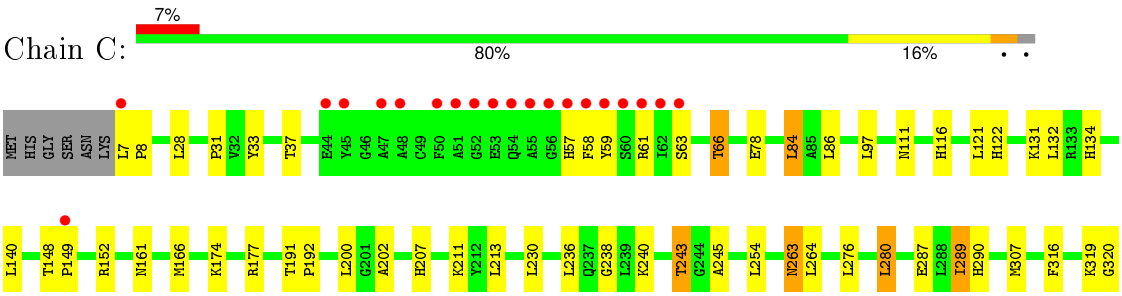
- Molecule 1: Methionine gamma-lyase

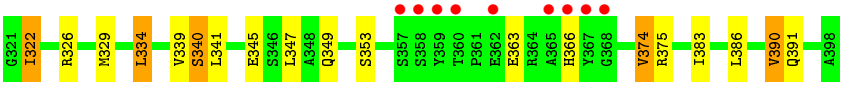
Chain B:



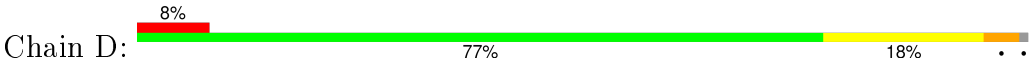
- Molecule 1: Methionine gamma-lyase

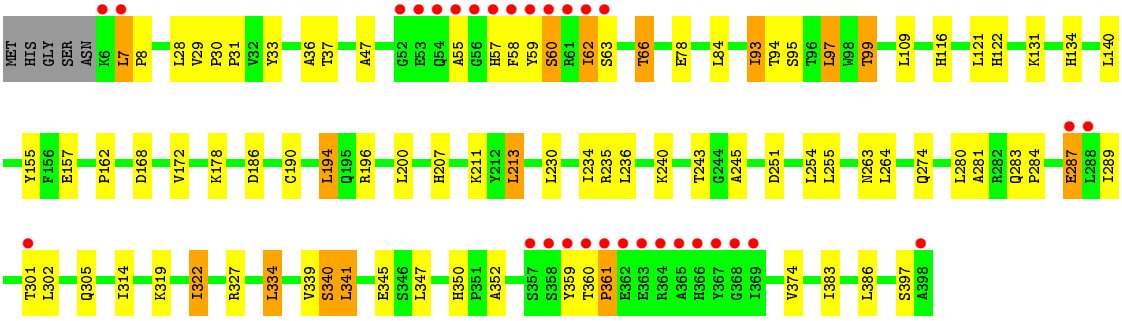
Chain C:





- Molecule 1: Methionine gamma-lyase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	153.94Å 153.44Å 80.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 29.34 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.0 (30.00-2.30) 99.0 (29.34-2.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.96 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.189 , 0.231 0.188 , 0.228	Depositor DCC
R_{free} test set	4253 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	21.8	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 38.5	EDS
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 84817 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12350	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 3.65% 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: LLP, 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	0.62	0/3019	0.74	2/4097 (0.0%)
1	B	0.67	0/3037	0.74	2/4121 (0.0%)
1	C	0.62	0/3010	0.73	2/4086 (0.0%)
1	D	0.59	0/3019	0.71	1/4097 (0.0%)
All	All	0.62	0/12085	0.73	7/16401 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	230	LEU	CA-CB-CG	5.38	127.67	115.30
1	B	280	LEU	CA-CB-CG	5.30	127.49	115.30
1	B	200	LEU	CA-CB-CG	5.20	127.25	115.30
1	D	251	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	233	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	C	280	LEU	CA-CB-CG	5.12	127.08	115.30
1	C	322	ILE	CB-CA-C	-5.10	101.40	111.60

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	2979	0	2941	45	0
1	B	2997	0	2955	53	0
1	C	2970	0	2929	51	0
1	D	2979	0	2942	56	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	99	0	0	6	0
3	B	115	0	0	7	0
3	C	110	0	0	7	0
3	D	81	0	0	3	0
All	All	12350	0	11767	191	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 8.

All (191) 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:362:GLU:O	1:B:363:GLU:HB2	1.51	1.09
1:B:327:ARG:HG2	1:B:327:ARG:HH21	1.15	1.08
1:B:363:GLU:O	1:B:364:ARG:HG3	1.55	1.05
1:A:93:ILE:HG21	3:A:428:HOH:O	1.57	1.02
1:A:284:PRO:O	1:A:319:LYS:HE2	1.64	0.97
1:B:45:TYR:HB3	3:B:449:HOH:O	1.68	0.92
1:A:57:HIS:HA	1:A:63:SER:HB2	1.54	0.89
1:D:287:GLU:HG2	1:D:319:LYS:HG3	1.54	0.89
1:D:33:TYR:H	1:D:66:THR:HG21	1.38	0.86
1:B:327:ARG:NH2	1:B:327:ARG:HG2	1.89	0.84
1:C:33:TYR:H	1:C:66:THR:CG2	1.90	0.83
1:D:33:TYR:H	1:D:66:THR:CG2	1.92	0.83
1:C:7:LEU:HD13	1:C:8:PRO:O	1.79	0.83
1:B:363:GLU:O	1:B:364:ARG:CG	2.30	0.80
1:A:33:TYR:H	1:A:66:THR:HG21	1.47	0.78
1:D:99:THR:HG21	1:D:234:ILE:HA	1.66	0.78
1:C:243:THR:HG22	1:C:245:ALA:H	1.49	0.77
1:A:360:THR:HB	1:A:361:PRO:HD2	1.66	0.77
1:A:360:THR:HB	1:A:361:PRO:CD	2.15	0.77
1:A:122:HIS:NE2	1:A:134:HIS:HE1	1.83	0.76
1:B:320:GLY:HA3	3:B:414:HOH:O	1.85	0.76
1:A:236:LEU:O	1:A:240:LYS:HE3	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:GLY:HA3	1:B:350:HIS:CE1	2.19	0.75
1:C:7:LEU:HD13	1:C:7:LEU:C	2.07	0.75
1:C:66:THR:HB	3:C:469:HOH:O	1.86	0.75
1:A:284:PRO:HB3	3:A:451:HOH:O	1.87	0.74
1:D:162:PRO:HD2	3:D:439:HOH:O	1.87	0.73
1:A:284:PRO:HD2	1:A:285:GLN:OE1	1.88	0.73
1:B:58:PHE:H	1:B:58:PHE:HD1	1.36	0.73
1:C:33:TYR:H	1:C:66:THR:HG21	1.52	0.73
1:B:323:GLY:O	1:B:327:ARG:HD3	1.89	0.73
1:A:33:TYR:H	1:A:66:THR:CG2	2.02	0.72
1:C:319:LYS:HA	3:C:422:HOH:O	1.89	0.71
1:A:78:GLU:OE2	1:A:207:HIS:HE1	1.72	0.71
1:D:281:ALA:HA	1:D:289:ILE:HD11	1.70	0.71
1:B:339:VAL:O	1:B:340:SER:HB2	1.90	0.70
1:D:243:THR:HG22	1:D:245:ALA:H	1.56	0.70
1:D:78:GLU:OE2	1:D:207:HIS:HE1	1.75	0.70
1:A:95:SER:O	1:A:99:THR:CG2	2.41	0.69
1:B:364:ARG:O	1:B:368:GLY:N	2.25	0.68
1:C:116:HIS:CE1	1:D:240:LYS:HD2	2.27	0.68
1:C:339:VAL:O	1:C:340:SER:CB	2.40	0.68
1:D:33:TYR:HB2	1:D:66:THR:HG23	1.75	0.68
1:C:148:THR:HB	1:C:149:PRO:HD2	1.76	0.67
1:D:58:PHE:N	1:D:63:SER:OG	2.27	0.66
1:B:211:LLP:HD3	1:B:341:LEU:HG	1.78	0.66
1:A:28:LEU:HD11	1:D:345:GLU:HG3	1.78	0.66
1:B:362:GLU:O	1:B:363:GLU:CB	2.32	0.65
1:A:99:THR:HG21	1:A:234:ILE:HA	1.78	0.65
1:A:243:THR:HG22	1:A:245:ALA:H	1.61	0.65
1:B:58:PHE:CD1	1:B:58:PHE:N	2.65	0.65
1:A:78:GLU:OE2	1:A:207:HIS:CE1	2.50	0.64
1:D:78:GLU:OE2	1:D:207:HIS:CE1	2.52	0.62
1:C:339:VAL:O	1:C:340:SER:HB3	1.99	0.61
1:A:95:SER:O	1:A:99:THR:HG22	2.00	0.61
1:C:122:HIS:NE2	1:C:134:HIS:HE1	1.99	0.61
1:B:327:ARG:HH21	1:B:327:ARG:CG	2.02	0.59
1:D:211:LLP:HD3	1:D:341:LEU:HG	1.85	0.59
1:B:122:HIS:NE2	1:B:134:HIS:HE1	2.02	0.58
1:C:263:ASN:HD22	1:C:263:ASN:H	1.49	0.58
1:D:95:SER:O	1:D:99:THR:CG2	2.52	0.58
1:D:236:LEU:O	1:D:240:LYS:HG2	2.04	0.57
1:D:95:SER:O	1:D:99:THR:HG22	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:339:VAL:O	1:D:340:SER:CB	2.53	0.57
1:A:62:ILE:CG2	1:A:235:ARG:HD3	2.35	0.57
1:C:7:LEU:CD1	1:C:8:PRO:O	2.53	0.56
1:D:360:THR:HB	1:D:361:PRO:HD2	1.87	0.56
1:A:339:VAL:O	1:A:340:SER:CB	2.53	0.56
1:D:93:ILE:HD12	1:D:97:LEU:HD22	1.88	0.56
1:B:320:GLY:CA	3:B:414:HOH:O	2.49	0.56
1:B:28:LEU:HD11	1:C:345:GLU:HG3	1.86	0.56
1:B:359:TYR:HB2	1:B:364:ARG:NH1	2.22	0.55
1:A:233:ARG:HD2	3:A:441:HOH:O	2.06	0.55
1:B:49:CYS:HB3	3:B:510:HOH:O	2.07	0.55
1:C:349:GLN:HE21	1:C:375:ARG:CZ	2.21	0.54
1:C:7:LEU:CD1	1:C:7:LEU:C	2.75	0.54
1:C:316:PHE:CE1	1:C:374:VAL:HG22	2.43	0.54
1:B:363:GLU:C	1:B:364:ARG:CG	2.75	0.54
1:C:349:GLN:HE21	1:C:375:ARG:NH2	2.06	0.53
1:D:62:ILE:HG23	1:D:235:ARG:HD3	1.89	0.53
1:C:240:LYS:HD2	1:D:116:HIS:HE1	1.73	0.53
1:A:93:ILE:CG2	3:A:428:HOH:O	2.34	0.52
1:B:243:THR:HG22	1:B:245:ALA:H	1.74	0.52
1:D:122:HIS:NE2	1:D:134:HIS:HE1	2.08	0.52
1:C:78:GLU:OE2	1:C:207:HIS:CE1	2.62	0.52
1:D:334:LEU:HD13	1:D:386:LEU:HD23	1.91	0.52
1:A:17:HIS:HD2	3:A:453:HOH:O	1.93	0.52
1:A:57:HIS:HA	1:A:63:SER:CB	2.35	0.51
1:A:211:LLP:NZ	1:A:211:LLP:O3	2.44	0.51
1:B:95:SER:OG	1:B:243:THR:HG21	2.09	0.51
1:D:211:LLP:NZ	1:D:211:LLP:O3	2.42	0.51
1:B:17:HIS:HD2	3:B:461:HOH:O	1.94	0.51
1:C:211:LLP:NZ	1:C:211:LLP:O3	2.42	0.51
1:D:157:GLU:HG2	1:D:186:ASP:HB3	1.93	0.51
1:B:78:GLU:OE2	1:B:207:HIS:HE1	1.93	0.51
1:B:363:GLU:C	1:B:365:ALA:H	2.14	0.50
1:C:243:THR:CG2	1:C:245:ALA:H	2.23	0.50
1:A:61:ARG:HG3	1:A:246:VAL:CG2	2.41	0.50
1:A:238:GLY:O	1:A:243:THR:HB	2.12	0.50
1:C:33:TYR:HB2	1:C:66:THR:HG23	1.93	0.50
1:B:339:VAL:O	1:B:340:SER:CB	2.59	0.50
1:B:211:LLP:NZ	1:B:211:LLP:O3	2.45	0.50
1:C:116:HIS:HE1	1:D:240:LYS:HD2	1.72	0.49
1:B:345:GLU:HG2	1:C:28:LEU:HD21	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:339:VAL:O	1:D:340:SER:HB3	2.11	0.49
1:D:350:HIS:CE1	1:D:352:ALA:HB3	2.47	0.49
1:C:7:LEU:O	1:C:7:LEU:HD13	2.12	0.49
1:C:191:THR:HB	1:C:192:PRO:HD2	1.93	0.49
1:A:345:GLU:HG3	1:D:28:LEU:HD11	1.95	0.49
1:D:207:HIS:HD2	3:D:400:HOH:O	1.96	0.49
1:C:326:ARG:HD2	3:C:425:HOH:O	2.12	0.49
1:B:78:GLU:OE2	1:B:207:HIS:CE1	2.66	0.49
1:A:95:SER:O	1:A:99:THR:HG23	2.12	0.49
1:A:243:THR:CG2	1:A:245:ALA:H	2.24	0.49
1:B:321:GLY:O	1:B:322:ILE:C	2.52	0.48
1:B:327:ARG:NH2	1:B:327:ARG:CG	2.68	0.48
1:D:284:PRO:O	1:D:319:LYS:HE3	2.12	0.48
1:A:206:VAL:HG12	1:A:224:VAL:HG22	1.95	0.48
1:C:329:MET:HE1	1:C:349:GLN:HA	1.95	0.48
1:C:7:LEU:O	1:C:7:LEU:CD1	2.62	0.47
1:D:36:ALA:O	1:D:60:SER:HB2	2.14	0.47
1:C:240:LYS:HD2	1:D:116:HIS:CE1	2.49	0.47
1:D:59:TYR:O	1:D:63:SER:N	2.47	0.47
1:D:302:LEU:HA	1:D:305:GLN:HE21	1.80	0.47
1:C:290:HIS:ND1	3:C:460:HOH:O	2.30	0.47
1:B:329:MET:HE1	1:B:349:GLN:HA	1.96	0.47
1:C:238:GLY:O	1:C:243:THR:HB	2.15	0.46
1:B:237:GLN:NE2	3:B:430:HOH:O	2.39	0.46
1:B:360:THR:O	1:B:362:GLU:O	2.34	0.46
1:D:243:THR:HG22	1:D:245:ALA:N	2.28	0.46
1:B:263:ASN:H	1:B:263:ASN:HD22	1.62	0.46
1:D:281:ALA:HA	1:D:289:ILE:CD1	2.43	0.46
1:B:362:GLU:HG3	1:B:363:GLU:N	2.31	0.46
1:C:61:ARG:NE	1:D:211:LLP:OP3	2.49	0.46
1:B:243:THR:CG2	1:B:245:ALA:H	2.28	0.46
1:B:8:PRO:O	1:B:13:ARG:HD3	2.16	0.46
1:D:66:THR:HB	3:D:410:HOH:O	2.15	0.46
1:D:168:ASP:O	1:D:172:VAL:HG23	2.16	0.46
1:A:93:ILE:HG13	1:A:94:THR:N	2.30	0.46
1:A:322:ILE:HG13	1:A:322:ILE:H	1.46	0.46
1:B:31:PRO:HB2	1:D:31:PRO:HB2	1.97	0.45
3:C:450:HOH:O	1:D:339:VAL:HG22	2.15	0.45
1:C:287:GLU:HB2	1:C:319:LYS:HG2	1.99	0.45
1:C:334:LEU:HD13	1:C:386:LEU:HD23	1.98	0.45
1:A:334:LEU:HD13	1:A:386:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:TYR:CE1	1:B:342:GLY:HA2	2.52	0.44
1:C:353:SER:O	1:D:47:ALA:HB2	2.16	0.44
1:C:166:MET:HE1	1:C:307:MET:SD	2.57	0.44
1:A:33:TYR:CE2	1:C:31:PRO:HG3	2.51	0.44
1:B:323:GLY:O	1:B:327:ARG:CD	2.63	0.44
1:C:57:HIS:CD2	1:C:63:SER:OG	2.70	0.44
1:C:78:GLU:OE2	1:C:207:HIS:HE1	2.00	0.44
1:D:93:ILE:HG13	1:D:94:THR:N	2.33	0.44
1:D:283:GLN:HA	1:D:284:PRO:HD2	1.85	0.43
1:C:386:LEU:O	1:C:390:VAL:HG13	2.19	0.43
1:C:236:LEU:O	1:C:240:LYS:HE3	2.18	0.43
1:B:161:ASN:HA	1:B:162:PRO:HA	1.83	0.43
1:A:214:SER:HB2	1:A:219:ILE:HD11	1.99	0.43
1:C:59:TYR:HE1	1:D:340:SER:HB2	1.84	0.43
1:B:335:PHE:CD1	1:B:346:SER:HB3	2.54	0.43
1:D:33:TYR:N	1:D:66:THR:HG21	2.20	0.42
1:D:57:HIS:HB2	1:D:63:SER:O	2.19	0.42
1:D:327:ARG:NH2	1:D:397:SER:O	2.51	0.42
1:B:152:ARG:NH2	1:B:180:GLY:O	2.53	0.42
1:A:327:ARG:HB3	1:A:397:SER:HA	2.02	0.42
1:D:7:LEU:N	1:D:8:PRO:HD3	2.34	0.42
1:A:330:ASN:OD1	1:B:43:VAL:HG22	2.19	0.42
1:A:111:ASN:HD22	1:A:134:HIS:HB3	1.84	0.42
1:B:347:LEU:HB2	1:B:377:SER:HB3	2.01	0.42
1:B:350:HIS:NE2	1:B:352:ALA:HB3	2.35	0.41
1:C:289:ILE:H	1:C:289:ILE:HD12	1.84	0.41
1:C:320:GLY:N	3:C:422:HOH:O	2.35	0.41
1:C:161:ASN:HA	1:C:161:ASN:HD22	1.56	0.41
1:C:202:ALA:O	3:C:506:HOH:O	2.22	0.41
1:D:29:VAL:HA	1:D:30:PRO:HD3	1.92	0.41
1:A:383:ILE:HG13	3:A:417:HOH:O	2.20	0.41
1:D:109:LEU:HA	1:D:155:TYR:O	2.19	0.41
1:B:316:PHE:CE1	1:B:374:VAL:HG22	2.55	0.41
1:A:111:ASN:HA	1:A:111:ASN:HD22	1.73	0.41
1:A:211:LLP:HD3	1:A:341:LEU:HG	2.02	0.41
1:A:61:ARG:HG3	1:A:246:VAL:HG22	2.02	0.41
1:A:89:GLY:O	1:A:93:ILE:HG23	2.21	0.41
1:B:13:ARG:NH2	3:B:435:HOH:O	2.51	0.41
1:D:190:CYS:O	1:D:194:LEU:HB2	2.21	0.41
1:C:276:LEU:HA	1:C:276:LEU:HD23	1.94	0.41
1:C:84:LEU:HD13	1:C:86:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:THR:HG21	1:B:262:LEU:HD11	2.03	0.41
1:B:110:GLY:O	1:B:134:HIS:HD2	2.04	0.40
1:A:327:ARG:NH2	1:A:397:SER:O	2.54	0.40
1:D:196:ARG:NH1	1:D:196:ARG:HG3	2.36	0.40
1:D:213:LEU:HB3	1:D:255:LEU:HD11	2.04	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	390/398 (98%)	375 (96%)	12 (3%)	3 (1%)	24	27
1	B	393/398 (99%)	377 (96%)	13 (3%)	3 (1%)	24	27
1	C	389/398 (98%)	374 (96%)	14 (4%)	1 (0%)	46	57
1	D	390/398 (98%)	371 (95%)	12 (3%)	7 (2%)	11	9
All	All	1562/1592 (98%)	1497 (96%)	51 (3%)	14 (1%)	21	24

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	340	SER
1	D	7	LEU
1	A	60	SER
1	A	340	SER
1	D	55	ALA
1	D	340	SER
1	B	322	ILE
1	D	287	GLU
1	D	322	ILE
1	A	53	GLU

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Mol	Chain	Res	Type
1	B	363	GLU
1	C	340	SER
1	D	62	ILE
1	D	361	PRO

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	302/306 (99%)	270 (89%)	32 (11%)	8 9
1	B	304/306 (99%)	274 (90%)	30 (10%)	10 11
1	C	301/306 (98%)	269 (89%)	32 (11%)	8 9
1	D	302/306 (99%)	273 (90%)	29 (10%)	10 12
All	All	1209/1224 (99%)	1086 (90%)	123 (10%)	9 10

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	37	THR
1	A	58	PHE
1	A	62	ILE
1	A	66	THR
1	A	84	LEU
1	A	93	ILE
1	A	97	LEU
1	A	99	THR
1	A	111	ASN
1	A	121	LEU
1	A	132	LEU
1	A	141	GLN
1	A	152	ARG
1	A	200	LEU
1	A	213	LEU
1	A	214	SER

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Mol	Chain	Res	Type
1	A	243	THR
1	A	263	ASN
1	A	264	LEU
1	A	280	LEU
1	A	289	ILE
1	A	304	ARG
1	A	322	ILE
1	A	334	LEU
1	A	341	LEU
1	A	347	LEU
1	A	359	TYR
1	A	366	HIS
1	A	374	VAL
1	A	383	ILE
1	A	391	GLN
1	B	7	LEU
1	B	22	GLN
1	B	49	CYS
1	B	58	PHE
1	B	84	LEU
1	B	97	LEU
1	B	111	ASN
1	B	121	LEU
1	B	132	LEU
1	B	140	LEU
1	B	166	MET
1	B	178	LYS
1	B	200	LEU
1	B	213	LEU
1	B	230	LEU
1	B	243	THR
1	B	254	LEU
1	B	263	ASN
1	B	264	LEU
1	B	268	ARG
1	B	280	LEU
1	B	287	GLU
1	B	301	THR
1	B	304	ARG
1	B	327	ARG
1	B	333	GLN
1	B	334	LEU

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Mol	Chain	Res	Type
1	B	339	VAL
1	B	347	LEU
1	B	374	VAL
1	C	37	THR
1	C	58	PHE
1	C	66	THR
1	C	84	LEU
1	C	97	LEU
1	C	111	ASN
1	C	121	LEU
1	C	131	LYS
1	C	132	LEU
1	C	140	LEU
1	C	152	ARG
1	C	174	LYS
1	C	177	ARG
1	C	200	LEU
1	C	213	LEU
1	C	230	LEU
1	C	243	THR
1	C	254	LEU
1	C	263	ASN
1	C	264	LEU
1	C	280	LEU
1	C	289	ILE
1	C	322	ILE
1	C	334	LEU
1	C	341	LEU
1	C	347	LEU
1	C	363	GLU
1	C	366	HIS
1	C	374	VAL
1	C	383	ILE
1	C	390	VAL
1	C	391	GLN
1	D	37	THR
1	D	60	SER
1	D	66	THR
1	D	84	LEU
1	D	93	ILE
1	D	97	LEU
1	D	99	THR

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Mol	Chain	Res	Type
1	D	121	LEU
1	D	131	LYS
1	D	140	LEU
1	D	178	LYS
1	D	194	LEU
1	D	200	LEU
1	D	213	LEU
1	D	230	LEU
1	D	254	LEU
1	D	263	ASN
1	D	264	LEU
1	D	274	GLN
1	D	280	LEU
1	D	301	THR
1	D	314	ILE
1	D	322	ILE
1	D	334	LEU
1	D	341	LEU
1	D	347	LEU
1	D	359	TYR
1	D	374	VAL
1	D	383	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	111	ASN
1	A	134	HIS
1	A	207	HIS
1	A	250	HIS
1	A	263	ASN
1	A	333	GLN
1	B	5	ASN
1	B	17	HIS
1	B	68	ASN
1	B	111	ASN
1	B	116	HIS
1	B	134	HIS
1	B	207	HIS
1	B	250	HIS
1	B	274	GLN

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Mol	Chain	Res	Type
1	B	391	GLN
1	C	111	ASN
1	C	116	HIS
1	C	134	HIS
1	C	161	ASN
1	C	207	HIS
1	C	250	HIS
1	C	263	ASN
1	C	274	GLN
1	C	305	GLN
1	C	349	GLN
1	D	22	GLN
1	D	54	GLN
1	D	116	HIS
1	D	134	HIS
1	D	161	ASN
1	D	207	HIS
1	D	250	HIS
1	D	305	GLN
1	D	309	GLN
1	D	356	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)

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	LLP	A	211	1	23,24,25	2.17	5 (21%)	28,32,34	1.61	7 (25%)
1	LLP	B	211	1	23,24,25	2.44	7 (30%)	28,32,34	1.58	7 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	LLP	C	211	1	23,24,25	2.18	6 (26%)	28,32,34	1.52	5 (17%)
1	LLP	D	211	1	23,24,25	2.43	9 (39%)	28,32,34	1.46	6 (21%)

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
1	LLP	A	211	1	-	0/15/17/19	0/1/1/1
1	LLP	B	211	1	-	0/15/17/19	0/1/1/1
1	LLP	C	211	1	-	0/15/17/19	0/1/1/1
1	LLP	D	211	1	-	0/15/17/19	0/1/1/1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	211	LLP	C2'-C2	-5.12	1.40	1.50
1	C	211	LLP	C2'-C2	-4.11	1.42	1.50
1	B	211	LLP	C4-C4'	-4.04	1.39	1.46
1	A	211	LLP	C2'-C2	-3.89	1.42	1.50
1	D	211	LLP	C2'-C2	-3.58	1.43	1.50
1	B	211	LLP	C5'-C5	-3.47	1.41	1.50
1	D	211	LLP	C4-C4'	-3.05	1.41	1.46
1	C	211	LLP	C5'-C5	-2.96	1.42	1.50
1	D	211	LLP	C5'-C5	-2.86	1.42	1.50
1	A	211	LLP	C5'-C5	-2.58	1.43	1.50
1	D	211	LLP	P-OP3	-2.47	1.45	1.54
1	A	211	LLP	P-OP2	-2.47	1.45	1.54
1	B	211	LLP	C3-C2	-2.45	1.39	1.40
1	B	211	LLP	P-OP2	-2.42	1.46	1.54
1	D	211	LLP	P-OP2	-2.39	1.46	1.54
1	C	211	LLP	P-OP3	-2.13	1.47	1.54
1	C	211	LLP	P-OP2	-2.10	1.47	1.54
1	D	211	LLP	C3-C2	-2.03	1.39	1.40
1	B	211	LLP	C6-N1	2.38	1.39	1.34
1	A	211	LLP	C6-N1	3.02	1.40	1.34
1	D	211	LLP	CB-CA	3.57	1.57	1.53
1	C	211	LLP	C6-N1	3.75	1.42	1.34
1	D	211	LLP	C6-N1	3.86	1.42	1.34
1	B	211	LLP	C4'-NZ	6.85	1.47	1.27
1	C	211	LLP	C4'-NZ	7.13	1.48	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	211	LLP	C4'-NZ	7.13	1.48	1.27
1	A	211	LLP	C4'-NZ	7.31	1.49	1.27

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	211	LLP	OP4-P-OP1	-3.72	97.66	107.14
1	B	211	LLP	CE-NZ-C4'	-2.94	110.47	118.97
1	C	211	LLP	CE-NZ-C4'	-2.93	110.52	118.97
1	B	211	LLP	OP2-P-OP4	-2.91	98.18	106.56
1	B	211	LLP	O-C-CA	-2.82	118.14	125.49
1	A	211	LLP	O-C-CA	-2.80	118.20	125.49
1	A	211	LLP	CE-NZ-C4'	-2.75	111.02	118.97
1	D	211	LLP	C4-C4'-NZ	-2.69	110.11	125.06
1	C	211	LLP	O-C-CA	-2.61	118.68	125.49
1	D	211	LLP	OP2-P-OP4	-2.61	99.04	106.56
1	D	211	LLP	O-C-CA	-2.54	118.88	125.49
1	A	211	LLP	C3-C2-N1	-2.34	117.37	120.61
1	C	211	LLP	C3-C2-N1	-2.25	117.50	120.61
1	B	211	LLP	C3-C2-N1	-2.10	117.71	120.61
1	C	211	LLP	OP2-P-OP4	-2.09	100.56	106.56
1	B	211	LLP	C4-C4'-NZ	-2.08	113.47	125.06
1	C	211	LLP	OP4-P-OP1	-2.01	102.02	107.14
1	D	211	LLP	C2'-C2-N1	2.00	122.38	117.95
1	D	211	LLP	OP4-C5'-C5	2.10	112.47	108.99
1	A	211	LLP	OP3-P-OP1	2.10	117.36	110.58
1	B	211	LLP	C5'-C5-C4	2.13	125.05	121.47
1	A	211	LLP	OP4-C5'-C5	2.44	113.03	108.99
1	D	211	LLP	OP3-P-OP2	2.45	116.73	107.38
1	A	211	LLP	C5'-C5-C4	2.64	125.90	121.47
1	B	211	LLP	OP3-P-OP2	2.67	117.54	107.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	211	LLP	2	0
1	B	211	LLP	2	0
1	C	211	LLP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	211	LLP	3	0

5.5 Carbohydrates (i)

There are no carbohydrates 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	A	501	-	4,4,4	0.11	0	6,6,6	0.14	0
2	SO4	B	501	-	4,4,4	0.21	0	6,6,6	0.07	0
2	SO4	C	501	-	4,4,4	0.23	0	6,6,6	0.17	0
2	SO4	D	501	-	4,4,4	0.17	0	6,6,6	0.14	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	501	-	-	0/0/0/0	0/0/0/0
2	SO4	B	501	-	-	0/0/0/0	0/0/0/0
2	SO4	C	501	-	-	0/0/0/0	0/0/0/0
2	SO4	D	501	-	-	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.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	392/398 (98%)	0.10	30 (7%)	16	23	7, 20, 67, 88	0
1	B	395/398 (99%)	0.13	37 (9%)	11	16	6, 17, 73, 84	0
1	C	391/398 (98%)	-0.00	29 (7%)	17	25	6, 18, 62, 91	0
1	D	392/398 (98%)	0.28	31 (7%)	15	22	9, 26, 72, 90	0
All	All	1570/1592 (98%)	0.13	127 (8%)	15	21	6, 20, 68, 91	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	59	TYR	14.5
1	A	62	ILE	9.6
1	B	366	HIS	9.5
1	D	62	ILE	9.4
1	A	54	GLN	9.3
1	D	358	SER	9.2
1	C	52	GLY	9.2
1	B	51	ALA	9.1
1	D	52	GLY	8.7
1	C	53	GLU	8.6
1	B	55	ALA	8.5
1	C	55	ALA	8.4
1	B	368	GLY	8.4
1	C	51	ALA	8.3
1	B	54	GLN	7.7
1	A	52	GLY	7.7
1	D	61	ARG	7.3
1	C	54	GLN	7.1
1	B	58	PHE	7.1
1	D	365	ALA	6.9
1	A	58	PHE	6.9

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Mol	Chain	Res	Type	RSRZ
1	A	55	ALA	6.9
1	C	58	PHE	6.6
1	B	367	TYR	6.6
1	A	51	ALA	6.5
1	D	55	ALA	6.5
1	D	54	GLN	6.5
1	D	58	PHE	6.3
1	D	359	TYR	6.2
1	D	60	SER	6.2
1	B	360	THR	6.1
1	B	48	ALA	6.1
1	B	358	SER	5.9
1	A	53	GLU	5.7
1	A	47	ALA	5.7
1	A	59	TYR	5.4
1	A	60	SER	5.4
1	D	367	TYR	5.4
1	D	6	LYS	5.4
1	D	57	HIS	5.4
1	C	48	ALA	5.4
1	D	366	HIS	5.3
1	D	368	GLY	5.3
1	A	56	GLY	5.2
1	B	45	TYR	5.2
1	C	60	SER	5.2
1	C	45	TYR	5.1
1	B	63	SER	5.1
1	A	57	HIS	5.1
1	D	360	THR	5.0
1	A	61	ARG	5.0
1	B	59	TYR	4.9
1	B	62	ILE	4.8
1	D	56	GLY	4.8
1	C	359	TYR	4.7
1	A	50	PHE	4.7
1	D	53	GLU	4.7
1	D	363	GLU	4.7
1	A	367	TYR	4.6
1	D	362	GLU	4.6
1	A	6	LYS	4.6
1	B	56	GLY	4.5
1	B	49	CYS	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	362	GLU	4.5
1	A	359	TYR	4.5
1	C	57	HIS	4.4
1	B	47	ALA	4.4
1	A	48	ALA	4.4
1	A	398	ALA	4.3
1	A	366	HIS	4.2
1	C	63	SER	4.2
1	C	366	HIS	4.1
1	D	357	SER	4.1
1	C	59	TYR	4.1
1	C	367	TYR	4.0
1	B	359	TYR	3.9
1	B	361	PRO	3.9
1	B	52	GLY	3.8
1	B	398	ALA	3.8
1	C	358	SER	3.8
1	B	50	PHE	3.7
1	A	365	ALA	3.6
1	A	360	THR	3.5
1	B	320	GLY	3.5
1	C	50	PHE	3.5
1	A	45	TYR	3.4
1	A	362	GLU	3.3
1	A	358	SER	3.3
1	C	365	ALA	3.3
1	D	398	ALA	3.2
1	C	368	GLY	3.2
1	C	362	GLU	3.2
1	D	287	GLU	3.1
1	B	322	ILE	3.1
1	C	47	ALA	3.1
1	B	44	GLU	3.0
1	B	6	LYS	2.9
1	A	7	LEU	2.9
1	B	53	GLU	2.9
1	B	57	HIS	2.9
1	B	365	ALA	2.8
1	C	62	ILE	2.8
1	A	22	GLN	2.8
1	C	7	LEU	2.8
1	B	41	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	288	LEU	2.7
1	B	371	GLU	2.6
1	D	63	SER	2.6
1	C	61	ARG	2.6
1	C	149	PRO	2.6
1	C	44	GLU	2.6
1	B	321	GLY	2.5
1	D	361	PRO	2.5
1	D	7	LEU	2.5
1	A	361	PRO	2.4
1	B	364	ARG	2.4
1	B	43	VAL	2.4
1	D	364	ARG	2.4
1	C	56	GLY	2.3
1	A	363	GLU	2.3
1	B	357	SER	2.3
1	C	357	SER	2.2
1	A	63	SER	2.2
1	D	369	ILE	2.1
1	B	5	ASN	2.1
1	C	360	THR	2.0
1	D	301	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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. 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
1	LLP	C	211	24/25	0.97	0.13	-	9,14,15,17	0
1	LLP	D	211	24/25	0.97	0.12	-	12,19,21,22	0
1	LLP	A	211	24/25	0.98	0.14	-	9,15,19,20	0
1	LLP	B	211	24/25	0.97	0.11	-	8,11,14,15	0

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	C	501	5/5	0.81	0.31	4.58	90,90,91,91	0
2	SO4	B	501	5/5	0.84	0.21	0.99	94,94,94,94	0
2	SO4	D	501	5/5	0.87	0.21	0.31	90,90,90,91	0
2	SO4	A	501	5/5	0.91	0.15	-0.13	74,74,75,75	0

6.5 Other polymers

There are no such residues in this entry.