Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2023 – 11:44 AM JST

PDB ID	:	5X2V
Title	:	Crystal structure of Pseudomonas putida methionine gamma-lyase wild type without sulfate ion
Authors	:	Shiba, T.; Sato, D.; Harada, S.
Deposited on	:	2017-02-02
Resolution	:	2.40 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:

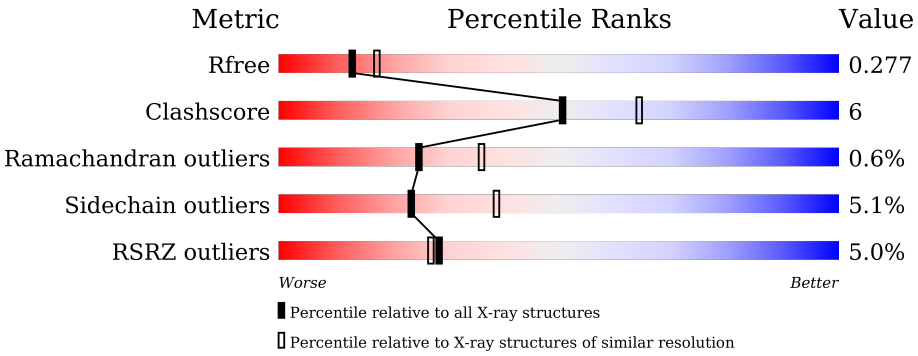
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.40 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 <=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	6% 80% 16%
1	B	398	4% 85% 12%
1	C	398	4% 83% 14%
1	D	398	5% 83% 15%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11939 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 L-methionine gamma-lyase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	P	S	0	0	0
			2966	1871	523	554	1	17			
1	B	392	Total	C	N	O	P	S	0	0	0
			2966	1871	523	554	1	17			
1	C	392	Total	C	N	O	P	S	0	0	0
			2966	1871	523	554	1	17			
1	D	396	Total	C	N	O	P	S	0	0	0
			2993	1886	529	560	1	17			

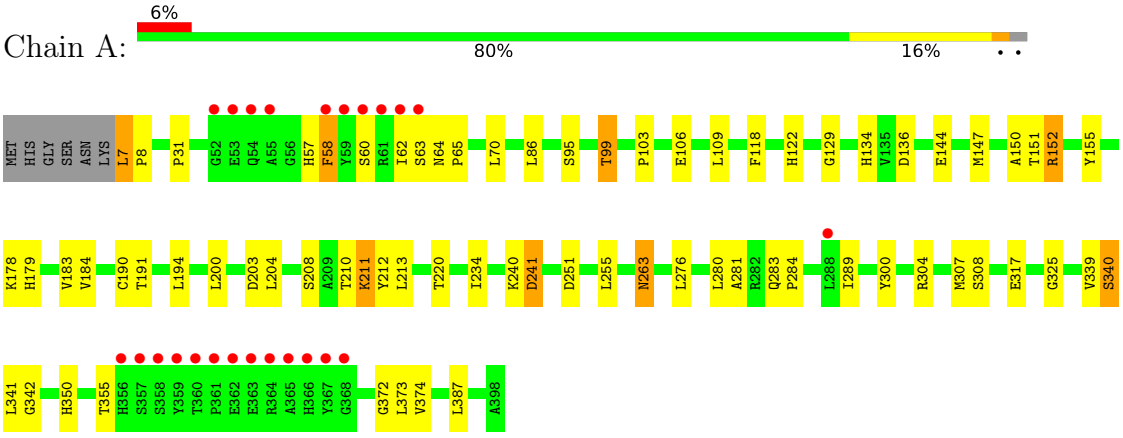
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	10	Total	O	0	0
			10	10		
2	B	12	Total	O	0	0
			12	12		
2	C	13	Total	O	0	0
			13	13		
2	D	13	Total	O	0	0
			13	13		

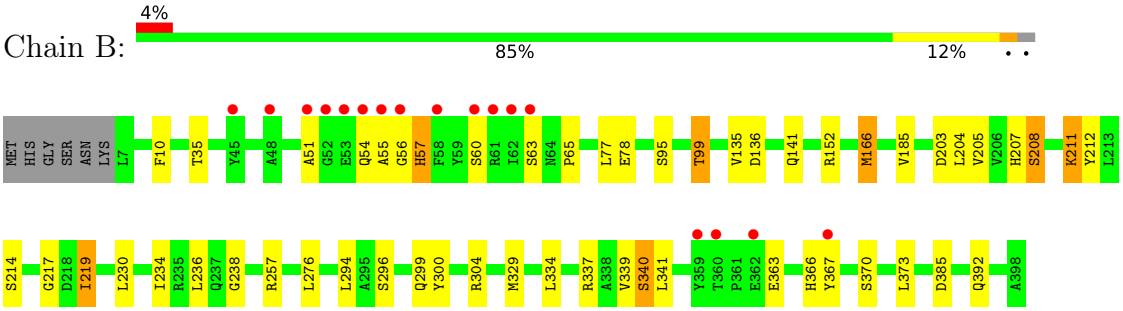
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

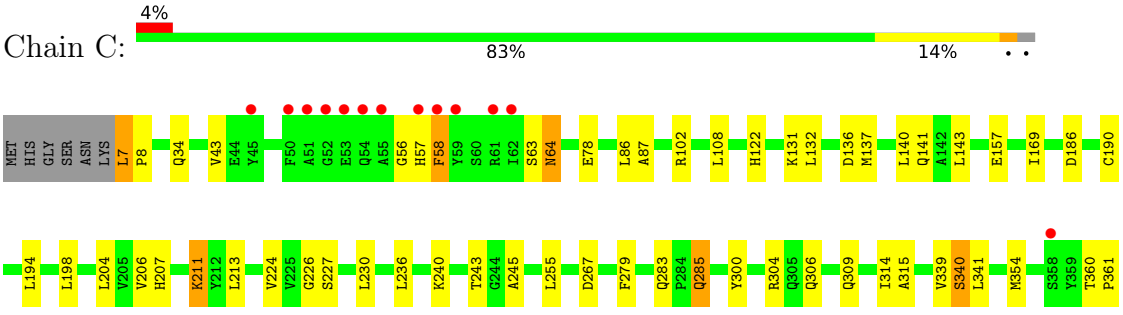
• Molecule 1: L-methionine gamma-lyase

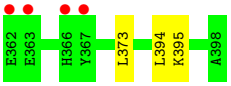


• Molecule 1: L-methionine gamma-lyase

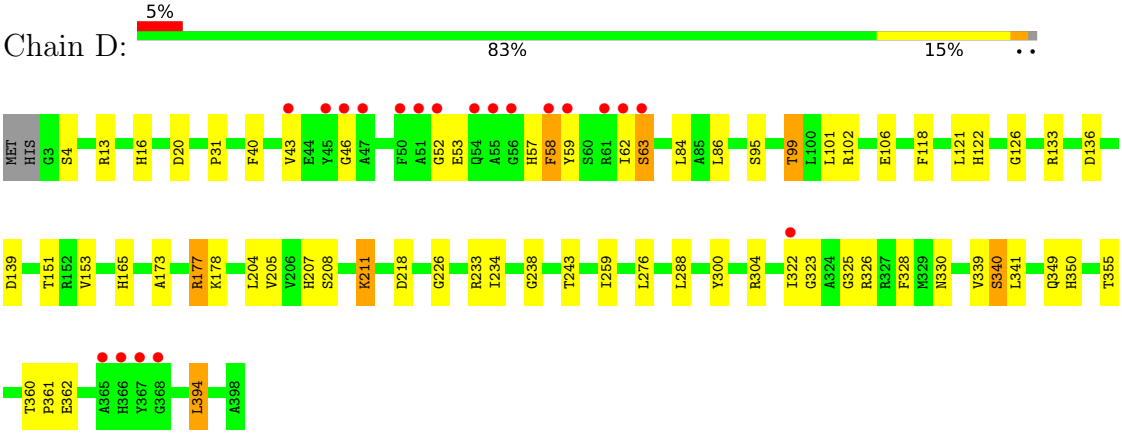


• Molecule 1: L-methionine gamma-lyase





• Molecule 1: L-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	154.22Å 153.53Å 80.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 29.31 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.0 (30.00-2.40) 98.1 (29.31-2.40)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.53 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.216 , 0.276 0.222 , 0.277	Depositor DCC
R_{free} test set	3731 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	21.3	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 5.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	11939	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: LLP

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	0/3005	0.79	2/4079 (0.0%)
1	B	0.69	1/3005 (0.0%)	0.86	4/4079 (0.1%)
1	C	0.63	0/3005	0.81	3/4079 (0.1%)
1	D	0.68	0/3032	0.83	6/4114 (0.1%)
All	All	0.66	1/12047 (0.0%)	0.82	15/16351 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	212	TYR	C-O	-5.50	1.12	1.23

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	56	GLY	N-CA-C	-9.91	88.33	113.10
1	C	267	ASP	CB-CG-OD2	7.54	125.09	118.30
1	D	13	ARG	NE-CZ-NH1	6.65	123.63	120.30
1	D	233	ARG	NE-CZ-NH1	6.51	123.55	120.30
1	B	208	SER	N-CA-C	-6.19	94.28	111.00
1	A	213	LEU	CB-CG-CD2	5.86	120.95	111.00
1	D	208	SER	N-CA-C	-5.55	96.00	111.00
1	D	102	ARG	NE-CZ-NH2	5.46	123.03	120.30
1	D	139	ASP	CB-CG-OD2	5.32	123.08	118.30
1	D	177	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	A	241	ASP	CB-CA-C	-5.09	100.21	110.40
1	B	385	ASP	CB-CG-OD2	5.08	122.87	118.30
1	C	102	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	C	213	LEU	CB-CG-CD1	5.03	119.55	111.00
1	B	257	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2966	0	2924	37	0
1	B	2966	0	2924	33	0
1	C	2966	0	2924	34	0
1	D	2993	0	2951	39	0
2	A	10	0	0	0	0
2	B	12	0	0	3	0
2	C	13	0	0	0	0
2	D	13	0	0	1	0
All	All	11939	0	11723	135	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 6.

All (135) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:THR:HG21	1:D:234:ILE:HA	1.64	0.79
1:A:95:SER:O	1:A:99:THR:HG23	1.85	0.76
1:B:57:HIS:HB3	1:B:63:SER:HB3	1.72	0.70
1:A:190:CYS:O	1:A:191:THR:HG23	1.93	0.68
1:B:57:HIS:CB	2:B:406:HOH:O	2.41	0.67
1:A:208:SER:OG	1:A:211:LLP:HE2	1.94	0.66
1:A:325:GLY:HA3	1:A:350:HIS:CE1	2.31	0.66
1:A:99:THR:HG21	1:A:234:ILE:HA	1.78	0.65
1:B:166:MET:H	1:B:299:GLN:HE22	1.43	0.65
1:B:57:HIS:CG	1:B:63:SER:OG	2.51	0.64
1:B:78:GLU:OE2	1:B:207:HIS:HE1	1.82	0.63
1:B:95:SER:O	1:B:99:THR:HG23	1.99	0.62
1:C:300:TYR:CZ	1:C:304:ARG:HD2	2.34	0.62
1:B:99:THR:HG21	1:B:234:ILE:HA	1.83	0.61
1:C:236:LEU:O	1:C:240:LYS:HE3	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:GLN:HG3	1:D:218:ASP:O	2.02	0.59
1:D:84:LEU:HD23	1:D:86:LEU:HD11	1.83	0.59
1:B:54:GLN:HG3	1:B:54:GLN:O	2.03	0.58
1:D:339:VAL:O	1:D:340:SER:HB2	2.04	0.57
1:B:339:VAL:O	1:B:340:SER:CB	2.52	0.57
1:B:57:HIS:N	1:B:57:HIS:CD2	2.72	0.56
1:C:339:VAL:O	1:C:340:SER:CB	2.53	0.56
1:B:54:GLN:O	1:B:55:ALA:HB3	2.07	0.55
1:C:43:VAL:H	1:D:330:ASN:HD21	1.54	0.54
1:C:204:LEU:HD23	1:C:226:GLY:HA3	1.88	0.54
1:D:204:LEU:HD23	1:D:226:GLY:HA3	1.90	0.54
1:A:57:HIS:HD2	1:A:63:SER:C	2.11	0.54
1:D:300:TYR:CZ	1:D:304:ARG:HD2	2.43	0.54
1:B:57:HIS:HB3	2:B:406:HOH:O	2.05	0.53
1:B:57:HIS:HB2	2:B:406:HOH:O	2.08	0.53
1:A:184:VAL:HG22	1:A:204:LEU:HB2	1.89	0.53
1:B:208:SER:OG	1:B:211:LLP:OP1	2.25	0.53
1:B:57:HIS:HB3	1:B:63:SER:CB	2.38	0.53
1:B:78:GLU:OE2	1:B:207:HIS:CE1	2.61	0.52
1:C:243:THR:HG22	1:D:243:THR:HA	1.91	0.52
1:A:70:LEU:HD21	1:A:255:LEU:HD23	1.91	0.52
1:A:194:LEU:O	1:A:307:MET:HA	2.09	0.51
1:B:300:TYR:CZ	1:B:304:ARG:HD2	2.45	0.51
1:D:173:ALA:O	1:D:177:ARG:HG3	2.10	0.51
1:A:58:PHE:CZ	1:A:62:ILE:HG21	2.45	0.51
1:A:263:ASN:HD22	1:A:263:ASN:H	1.59	0.51
1:D:106:GLU:HB3	1:D:151:THR:HA	1.91	0.51
1:C:57:HIS:ND1	1:C:63:SER:OG	2.42	0.51
1:A:150:ALA:O	1:A:152:ARG:NH2	2.44	0.51
1:C:122:HIS:CE1	1:C:132:LEU:HD23	2.46	0.51
1:B:99:THR:HG22	1:B:238:GLY:CA	2.41	0.50
1:A:57:HIS:CD2	1:A:63:SER:OG	2.64	0.50
1:A:58:PHE:CE2	1:A:62:ILE:HG21	2.47	0.50
1:C:64:ASN:C	1:C:64:ASN:OD1	2.49	0.50
1:C:300:TYR:CE2	1:C:304:ARG:HD2	2.48	0.49
1:D:288:LEU:C	1:D:288:LEU:HD12	2.32	0.49
1:D:57:HIS:CD2	1:D:63:SER:OG	2.65	0.49
1:B:35:THR:O	1:B:35:THR:HG23	2.12	0.49
1:A:118:PHE:CE1	1:A:122:HIS:CD2	3.01	0.49
1:B:211:LLP:HD3	1:B:341:LEU:HG	1.95	0.49
1:D:95:SER:O	1:D:99:THR:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:118:PHE:CZ	1:D:122:HIS:CD2	3.01	0.49
1:C:78:GLU:OE2	1:C:207:HIS:NE2	2.45	0.48
1:A:106:GLU:HB3	1:A:151:THR:HA	1.94	0.48
1:D:58:PHE:CE2	1:D:62:ILE:HG21	2.48	0.48
1:B:339:VAL:O	1:B:340:SER:HB2	2.13	0.48
1:C:169:ILE:H	1:C:306:GLN:HE22	1.61	0.48
1:C:279:PHE:O	1:C:283:GLN:HG2	2.13	0.48
1:B:329:MET:HE3	1:B:337:ARG:HG2	1.96	0.48
1:A:317:GLU:HA	1:A:372:GLY:O	2.14	0.47
1:A:183:VAL:N	1:A:203:ASP:OD2	2.33	0.47
1:B:230:LEU:O	1:B:234:ILE:HG13	2.15	0.47
1:C:78:GLU:O	1:C:198:LEU:HD12	2.14	0.47
1:A:136:ASP:C	1:A:136:ASP:OD2	2.53	0.47
1:B:57:HIS:HE1	1:B:65:PRO:CD	2.27	0.46
1:A:190:CYS:C	1:A:191:THR:HG23	2.36	0.46
1:A:281:ALA:HA	1:A:289:ILE:HD11	1.97	0.46
1:A:95:SER:O	1:A:99:THR:CG2	2.60	0.46
1:A:300:TYR:CE2	1:A:304:ARG:HD2	2.51	0.46
1:C:255:LEU:HD12	1:C:255:LEU:O	2.15	0.46
1:C:157:GLU:CG	1:C:186:ASP:HB3	2.46	0.46
1:C:190:CYS:HB3	1:C:194:LEU:HB2	1.98	0.46
1:B:166:MET:H	1:B:299:GLN:NE2	2.13	0.45
1:B:367:TYR:CD1	1:B:367:TYR:O	2.70	0.45
1:C:211:LLP:HE3	1:D:59:TYR:OH	2.16	0.45
1:D:339:VAL:O	1:D:339:VAL:HG23	2.15	0.45
1:A:212:TYR:CE1	1:A:342:GLY:HA2	2.52	0.45
1:B:334:LEU:HD11	1:D:16:HIS:CD2	2.52	0.44
1:A:103:PRO:HA	1:A:129:GLY:O	2.17	0.44
1:C:194:LEU:HD22	1:C:309:GLN:HB2	2.00	0.44
1:A:339:VAL:O	1:A:340:SER:CB	2.66	0.44
1:C:360:THR:HB	1:C:361:PRO:HD2	2.00	0.43
1:D:211:LLP:O3	1:D:211:LLP:NZ	2.50	0.43
1:A:210:THR:HG23	1:A:220:THR:HA	1.98	0.43
1:C:58:PHE:N	1:C:58:PHE:CD2	2.86	0.43
1:A:109:LEU:HA	1:A:155:TYR:O	2.19	0.43
1:C:206:VAL:HG12	1:C:224:VAL:HG22	1.99	0.43
1:A:339:VAL:O	1:A:340:SER:HB3	2.19	0.43
1:D:99:THR:HG22	1:D:238:GLY:CA	2.49	0.43
1:D:322:ILE:HG23	1:D:323:GLY:N	2.33	0.43
1:C:354:MET:HG3	1:D:43:VAL:HG22	2.00	0.43
1:D:121:LEU:O	1:D:126:GLY:HA3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:PHE:CD1	1:D:58:PHE:N	2.87	0.43
1:D:40:PHE:CD2	1:D:46:GLY:HA2	2.53	0.42
1:D:325:GLY:O	1:D:326:ARG:C	2.56	0.42
1:A:57:HIS:CE1	1:A:65:PRO:HG3	2.54	0.42
1:B:99:THR:HG22	1:B:238:GLY:N	2.35	0.42
1:C:204:LEU:HD11	1:C:230:LEU:HD22	2.00	0.42
1:B:214:SER:HB2	1:B:219:ILE:HD11	2.01	0.42
1:C:157:GLU:HG3	1:C:186:ASP:HB3	2.01	0.42
1:D:101:LEU:HD21	1:D:153:VAL:CG2	2.50	0.42
1:D:259:ILE:O	1:D:259:ILE:HG22	2.19	0.42
1:C:314:ILE:HG22	1:C:315:ALA:N	2.35	0.42
1:D:101:LEU:HD21	1:D:153:VAL:HG23	2.01	0.42
1:A:144:GLU:OE1	1:A:179:HIS:NE2	2.51	0.42
1:C:87:ALA:HB3	1:C:245:ALA:HB1	2.01	0.41
1:C:354:MET:HG3	1:D:43:VAL:CG2	2.50	0.41
1:D:328:PHE:CE2	1:D:394:LEU:HD13	2.55	0.41
1:C:136:ASP:OD1	1:C:137:MET:N	2.54	0.41
1:D:325:GLY:HA3	1:D:350:HIS:CE1	2.56	0.41
1:A:276:LEU:CD2	1:A:387:LEU:HD23	2.50	0.41
1:B:203:ASP:O	1:B:204:LEU:HD23	2.20	0.41
1:D:207:HIS:HD2	2:D:401:HOH:O	2.01	0.41
1:A:7:LEU:HA	1:A:8:PRO:HD2	1.88	0.41
1:A:7:LEU:HD13	1:A:8:PRO:O	2.20	0.41
1:A:31:PRO:HB2	1:D:31:PRO:HB2	2.03	0.41
1:C:136:ASP:OD1	1:C:136:ASP:C	2.59	0.41
1:D:276:LEU:HD12	1:D:276:LEU:HA	1.83	0.41
1:D:360:THR:O	1:D:361:PRO:C	2.59	0.41
1:B:135:VAL:HG12	1:B:136:ASP:N	2.36	0.40
1:C:7:LEU:HA	1:C:8:PRO:HD2	1.99	0.40
1:A:58:PHE:N	1:A:58:PHE:CD1	2.89	0.40
1:A:283:GLN:HA	1:A:284:PRO:HD2	1.93	0.40
1:B:185:VAL:O	1:B:205:VAL:HA	2.21	0.40
1:C:394:LEU:HD23	1:C:394:LEU:HA	1.94	0.40
1:D:20:ASP:OD1	1:D:20:ASP:C	2.60	0.40
1:B:10:PHE:CE2	1:B:77:LEU:HD22	2.57	0.40
1:C:285:GLN:HE21	1:C:285:GLN:H	1.69	0.40
1:D:259:ILE:O	1:D:259:ILE:CG2	2.68	0.40
1:D:136:ASP:OD2	1:D:165:HIS:NE2	2.49	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	389/398 (98%)	359 (92%)	28 (7%)	2 (0%)	29	41
1	B	389/398 (98%)	359 (92%)	27 (7%)	3 (1%)	19	29
1	C	389/398 (98%)	363 (93%)	24 (6%)	2 (0%)	29	41
1	D	393/398 (99%)	377 (96%)	13 (3%)	3 (1%)	19	29
All	All	1560/1592 (98%)	1458 (94%)	92 (6%)	10 (1%)	25	36

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	340	SER
1	D	340	SER
1	A	147	MET
1	C	340	SER
1	D	53	GLU
1	B	217	GLY
1	A	340	SER
1	B	51	ALA
1	C	56	GLY
1	D	52	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	301/306 (98%)	281 (93%)	20 (7%)	16	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	301/306 (98%)	285 (95%)	16 (5%)	22 37
1	C	301/306 (98%)	287 (95%)	14 (5%)	26 42
1	D	304/306 (99%)	292 (96%)	12 (4%)	32 50
All	All	1207/1224 (99%)	1145 (95%)	62 (5%)	24 39

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	58	PHE
1	A	60	SER
1	A	64	ASN
1	A	86	LEU
1	A	99	THR
1	A	134	HIS
1	A	152	ARG
1	A	178	LYS
1	A	200	LEU
1	A	240	LYS
1	A	241	ASP
1	A	251	ASP
1	A	263	ASN
1	A	280	LEU
1	A	308	SER
1	A	341	LEU
1	A	355	THR
1	A	373	LEU
1	A	374	VAL
1	B	57	HIS
1	B	60	SER
1	B	99	THR
1	B	141	GLN
1	B	152	ARG
1	B	166	MET
1	B	219	ILE
1	B	236	LEU
1	B	276	LEU
1	B	294	LEU
1	B	296	SER
1	B	363	GLU
1	B	366	HIS

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Mol	Chain	Res	Type
1	B	370	SER
1	B	373	LEU
1	B	392	GLN
1	C	7	LEU
1	C	58	PHE
1	C	64	ASN
1	C	86	LEU
1	C	108	LEU
1	C	131	LYS
1	C	140	LEU
1	C	141	GLN
1	C	143	LEU
1	C	227	SER
1	C	285	GLN
1	C	341	LEU
1	C	373	LEU
1	C	395	LYS
1	D	4	SER
1	D	58	PHE
1	D	63	SER
1	D	99	THR
1	D	133	ARG
1	D	178	LYS
1	D	205	VAL
1	D	341	LEU
1	D	349	GLN
1	D	355	THR
1	D	362	GLU
1	D	394	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	HIS
1	A	122	HIS
1	A	134	HIS
1	A	161	ASN
1	A	207	HIS
1	A	237	GLN
1	A	250	HIS
1	A	263	ASN
1	A	309	GLN

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Mol	Chain	Res	Type
1	B	24	HIS
1	B	57	HIS
1	B	64	ASN
1	B	111	ASN
1	B	141	GLN
1	B	161	ASN
1	B	207	HIS
1	B	228	GLN
1	B	250	HIS
1	B	274	GLN
1	B	299	GLN
1	B	306	GLN
1	B	330	ASN
1	B	392	GLN
1	C	34	GLN
1	C	141	GLN
1	C	161	ASN
1	C	165	HIS
1	C	187	ASN
1	C	237	GLN
1	C	250	HIS
1	C	285	GLN
1	C	299	GLN
1	C	306	GLN
1	D	34	GLN
1	D	57	HIS
1	D	68	ASN
1	D	161	ASN
1	D	187	ASN
1	D	207	HIS
1	D	309	GLN
1	D	330	ASN

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	B	211	1	23,24,25	2.30	11 (47%)	25,32,34	1.70	7 (28%)
1	LLP	C	211	1	23,24,25	2.70	11 (47%)	25,32,34	1.49	1 (4%)
1	LLP	A	211	1	23,24,25	2.27	9 (39%)	25,32,34	1.59	7 (28%)
1	LLP	D	211	1	23,24,25	2.56	10 (43%)	25,32,34	1.78	6 (24%)

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	B	211	1	-	5/16/17/19	0/1/1/1
1	LLP	C	211	1	-	5/16/17/19	0/1/1/1
1	LLP	A	211	1	-	6/16/17/19	0/1/1/1
1	LLP	D	211	1	-	3/16/17/19	0/1/1/1

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	211	LLP	C3-C2	5.43	1.46	1.40
1	C	211	LLP	C4-C5	5.02	1.48	1.42
1	C	211	LLP	C3-C2	4.71	1.45	1.40
1	C	211	LLP	C4-C3	4.48	1.47	1.40
1	A	211	LLP	C4-C5	4.37	1.47	1.42
1	C	211	LLP	P-OP3	-4.33	1.38	1.54
1	B	211	LLP	C3-C2	4.29	1.45	1.40
1	C	211	LLP	C4'-NZ	4.22	1.41	1.27
1	A	211	LLP	C4'-NZ	4.20	1.41	1.27
1	B	211	LLP	P-OP3	-4.19	1.38	1.54
1	D	211	LLP	C4'-NZ	4.19	1.41	1.27
1	D	211	LLP	C4-C3	4.17	1.47	1.40
1	B	211	LLP	C4'-NZ	4.11	1.41	1.27
1	C	211	LLP	P-OP2	-4.04	1.39	1.54
1	D	211	LLP	C4-C5	4.03	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	211	LLP	P-OP1	-3.96	1.37	1.50
1	D	211	LLP	P-OP1	-3.92	1.37	1.50
1	D	211	LLP	P-OP2	-3.83	1.40	1.54
1	A	211	LLP	P-OP1	-3.69	1.38	1.50
1	A	211	LLP	C4-C3	3.63	1.46	1.40
1	B	211	LLP	P-OP1	-3.44	1.39	1.50
1	D	211	LLP	P-OP3	-3.39	1.41	1.54
1	A	211	LLP	C3-C2	3.37	1.44	1.40
1	B	211	LLP	P-OP2	-3.30	1.42	1.54
1	A	211	LLP	P-OP3	-3.16	1.42	1.54
1	A	211	LLP	O3-C3	-2.81	1.30	1.37
1	B	211	LLP	P-OP4	-2.71	1.51	1.60
1	B	211	LLP	C4-C3	2.65	1.44	1.40
1	B	211	LLP	C4-C5	2.54	1.45	1.42
1	D	211	LLP	P-OP4	-2.40	1.52	1.60
1	A	211	LLP	P-OP4	-2.31	1.52	1.60
1	C	211	LLP	C6-N1	-2.26	1.29	1.34
1	A	211	LLP	P-OP2	-2.21	1.46	1.54
1	C	211	LLP	CE-NZ	-2.21	1.42	1.46
1	D	211	LLP	O3-C3	-2.21	1.31	1.37
1	C	211	LLP	O3-C3	-2.16	1.31	1.37
1	B	211	LLP	CE-NZ	-2.16	1.42	1.46
1	B	211	LLP	O3-C3	-2.13	1.32	1.37
1	C	211	LLP	C4-C4'	2.13	1.50	1.46
1	D	211	LLP	CE-NZ	-2.07	1.42	1.46
1	B	211	LLP	C6-N1	-2.06	1.30	1.34

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	211	LLP	C3-C4-C5	-4.46	114.84	118.26
1	D	211	LLP	OP2-P-OP4	-3.88	96.40	106.73
1	D	211	LLP	CD-CE-NZ	3.50	119.50	110.93
1	A	211	LLP	C4-C4'-NZ	-3.40	108.71	124.31
1	D	211	LLP	C4-C3-C2	-3.33	118.12	120.19
1	B	211	LLP	OP4-P-OP1	-3.25	97.35	106.47
1	B	211	LLP	C3-C4-C5	-3.10	115.88	118.26
1	D	211	LLP	C4-C4'-NZ	-2.89	111.02	124.31
1	D	211	LLP	C3-C4-C5	-2.75	116.15	118.26
1	A	211	LLP	OP3-P-OP4	2.69	113.90	106.73
1	A	211	LLP	C3-C4-C5	-2.62	116.25	118.26
1	D	211	LLP	C6-N1-C2	2.61	124.00	119.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	211	LLP	C4-C3-C2	-2.59	118.59	120.19
1	B	211	LLP	OP3-P-OP2	2.54	117.36	107.64
1	A	211	LLP	C4-C3-C2	-2.51	118.64	120.19
1	A	211	LLP	OP3-P-OP2	2.46	117.03	107.64
1	A	211	LLP	OP4-P-OP1	-2.28	100.07	106.47
1	B	211	LLP	CD-CE-NZ	2.15	116.19	110.93
1	B	211	LLP	C4-C4'-NZ	-2.14	114.49	124.31
1	A	211	LLP	OP4-C5'-C5	2.11	113.38	109.35
1	B	211	LLP	CE-NZ-C4'	-2.01	112.72	118.90

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	211	LLP	C4-C4'-NZ-CE
1	A	211	LLP	O-C-CA-CB
1	B	211	LLP	C4-C4'-NZ-CE
1	B	211	LLP	N-CA-CB-CG
1	B	211	LLP	O-C-CA-CB
1	B	211	LLP	CG-CD-CE-NZ
1	C	211	LLP	C4-C4'-NZ-CE
1	C	211	LLP	O-C-CA-CB
1	D	211	LLP	O-C-CA-CB
1	D	211	LLP	C4-C4'-NZ-CE
1	A	211	LLP	CG-CD-CE-NZ
1	A	211	LLP	CD-CE-NZ-C4'
1	C	211	LLP	CG-CD-CE-NZ
1	A	211	LLP	N-CA-CB-CG
1	D	211	LLP	N-CA-CB-CG
1	B	211	LLP	CD-CE-NZ-C4'
1	A	211	LLP	C3-C4-C4'-NZ
1	C	211	LLP	CD-CE-NZ-C4'
1	C	211	LLP	N-CA-CB-CG

There are no ring outliers.

4 monomers are involved in 5 short contacts:

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	391/398 (98%)	-0.21	24 (6%)	21	20	12, 27, 90, 148	0
1	B	391/398 (98%)	-0.42	17 (4%)	35	33	10, 21, 77, 116	0
1	C	391/398 (98%)	-0.38	17 (4%)	35	33	12, 22, 80, 121	0
1	D	395/398 (99%)	-0.30	20 (5%)	28	26	8, 20, 77, 121	0
All	All	1568/1592 (98%)	-0.33	78 (4%)	28	27	8, 22, 80, 148	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	59	TYR	12.0
1	A	61	ARG	10.7
1	A	62	ILE	8.4
1	D	366	HIS	7.9
1	A	60	SER	7.2
1	B	55	ALA	6.7
1	C	62	ILE	6.5
1	D	52	GLY	6.4
1	D	59	TYR	6.3
1	C	51	ALA	5.9
1	C	54	GLN	5.5
1	D	55	ALA	5.4
1	A	55	ALA	5.3
1	C	59	TYR	5.1
1	C	55	ALA	5.1
1	B	54	GLN	5.0
1	C	367	TYR	4.9
1	A	54	GLN	4.8
1	C	52	GLY	4.6
1	D	62	ILE	4.5
1	D	367	TYR	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	58	PHE	4.1
1	D	51	ALA	4.1
1	A	362	GLU	4.0
1	A	360	THR	4.0
1	A	53	GLU	3.9
1	B	58	PHE	3.7
1	D	50	PHE	3.5
1	A	358	SER	3.5
1	C	53	GLU	3.5
1	B	52	GLY	3.4
1	A	366	HIS	3.4
1	C	366	HIS	3.4
1	A	52	GLY	3.4
1	B	45	TYR	3.4
1	D	47	ALA	3.4
1	C	57	HIS	3.3
1	D	54	GLN	3.3
1	B	53	GLU	3.2
1	D	58	PHE	3.2
1	D	56	GLY	3.2
1	C	58	PHE	3.2
1	A	357	SER	3.1
1	B	367	TYR	3.1
1	D	45	TYR	3.1
1	B	51	ALA	3.1
1	C	45	TYR	3.1
1	C	363	GLU	3.0
1	B	359	TYR	3.0
1	A	63	SER	3.0
1	B	60	SER	3.0
1	A	364	ARG	2.9
1	A	363	GLU	2.8
1	A	367	TYR	2.7
1	C	61	ARG	2.7
1	D	368	GLY	2.5
1	D	46	GLY	2.5
1	B	62	ILE	2.4
1	B	56	GLY	2.4
1	B	362	GLU	2.4
1	A	356	HIS	2.4
1	A	368	GLY	2.4
1	B	61	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	48	ALA	2.3
1	A	288	LEU	2.2
1	D	61	ARG	2.2
1	D	63	SER	2.2
1	D	43	VAL	2.1
1	C	358	SER	2.1
1	A	359	TYR	2.1
1	D	365	ALA	2.1
1	A	361	PRO	2.1
1	C	50	PHE	2.1
1	A	365	ALA	2.0
1	B	360	THR	2.0
1	B	63	SER	2.0
1	D	322	ILE	2.0
1	C	362	GLU	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. 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	B-factors(Å^2)	Q<0.9
1	LLP	A	211	24/25	0.97	0.11	17,20,24,27	0
1	LLP	B	211	24/25	0.97	0.11	16,21,23,24	0
1	LLP	C	211	24/25	0.98	0.09	14,18,20,22	0
1	LLP	D	211	24/25	0.98	0.10	12,18,25,26	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.