Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2024 – 11:47 AM EDT

PDB ID	:	5HUQ
Title	:	A tethered niacin-derived pincer complex with a nickel-carbon bond in lactate racemase
Authors	:	Desguin, B.; Zhang, T.; Soumillion, P.; Hols, P.; Hu, J.; Hausinger, R.P.
Deposited on	:	2016-01-27
Resolution	:	3.00 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:

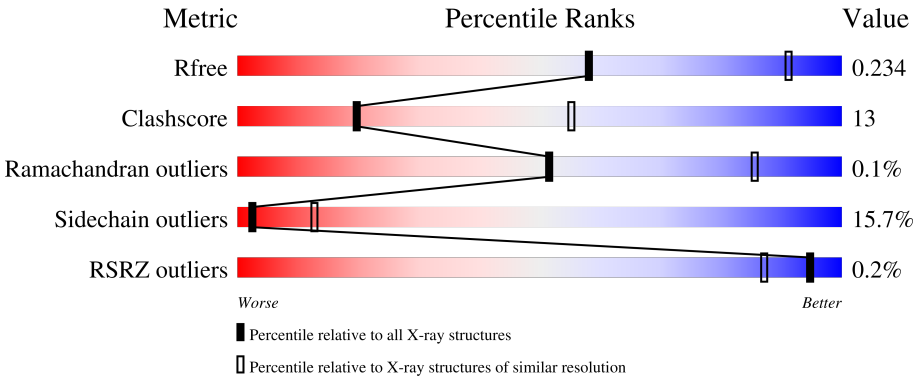
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 <=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	433	71% 22% 6%
1	B	433	70% 24% 6%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	505	-	-	-	X
3	SO4	A	507	-	-	-	X
3	SO4	B	513	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6780 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.

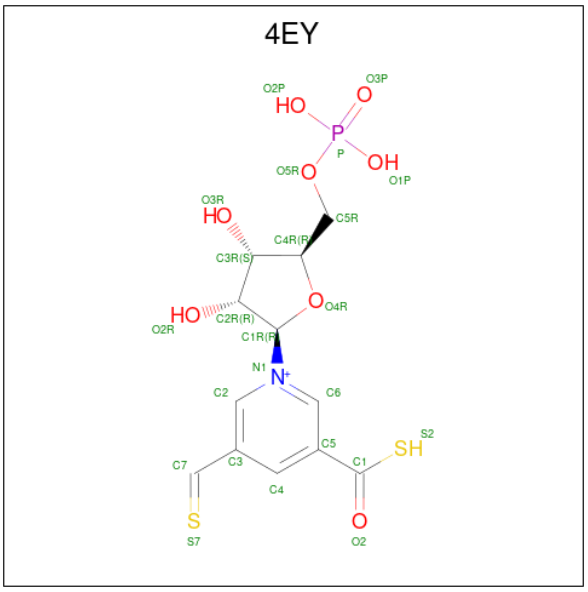
- Molecule 1 is a protein called Lactate racemization operon protein LarA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	433	Total	C	N	O	S	0	0	0
			3310	2084	576	636	14			
1	B	432	Total	C	N	O	S	0	0	0
			3306	2079	574	639	14			

There are 22 discrepancies between the modelled and reference sequences:

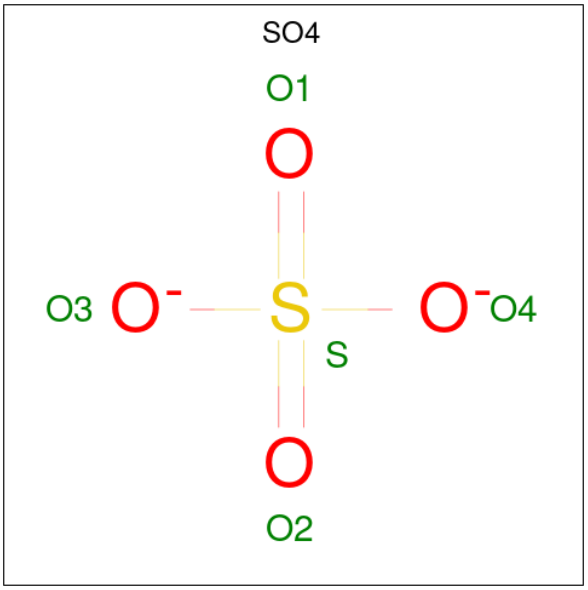
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP A0A0G9FER8
A	219	SER	PRO	conflict	UNP A0A0G9FER8
A	425	ALA	-	expression tag	UNP A0A0G9FER8
A	426	SER	-	expression tag	UNP A0A0G9FER8
A	427	TRP	-	expression tag	UNP A0A0G9FER8
A	428	SER	-	expression tag	UNP A0A0G9FER8
A	429	HIS	-	expression tag	UNP A0A0G9FER8
A	430	PRO	-	expression tag	UNP A0A0G9FER8
A	431	GLN	-	expression tag	UNP A0A0G9FER8
A	432	PHE	-	expression tag	UNP A0A0G9FER8
A	433	GLU	-	expression tag	UNP A0A0G9FER8
B	1	SER	-	expression tag	UNP A0A0G9FER8
B	219	SER	PRO	conflict	UNP A0A0G9FER8
B	425	ALA	-	expression tag	UNP A0A0G9FER8
B	426	SER	-	expression tag	UNP A0A0G9FER8
B	427	TRP	-	expression tag	UNP A0A0G9FER8
B	428	SER	-	expression tag	UNP A0A0G9FER8
B	429	HIS	-	expression tag	UNP A0A0G9FER8
B	430	PRO	-	expression tag	UNP A0A0G9FER8
B	431	GLN	-	expression tag	UNP A0A0G9FER8
B	432	PHE	-	expression tag	UNP A0A0G9FER8
B	433	GLU	-	expression tag	UNP A0A0G9FER8

- Molecule 2 is 3-methanethioyl-1-(5-O-phosphono-beta-D-ribofuranosyl)-5-(sulfanylcarbonyl) pyridin-1-ium (three-letter code: 4EY) (formula: $C_{12}H_{15}NO_8PS_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			24	12	1	8	1	2		
2	B	1	Total	C	N	O	P	S	0	0
			24	12	1	8	1	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

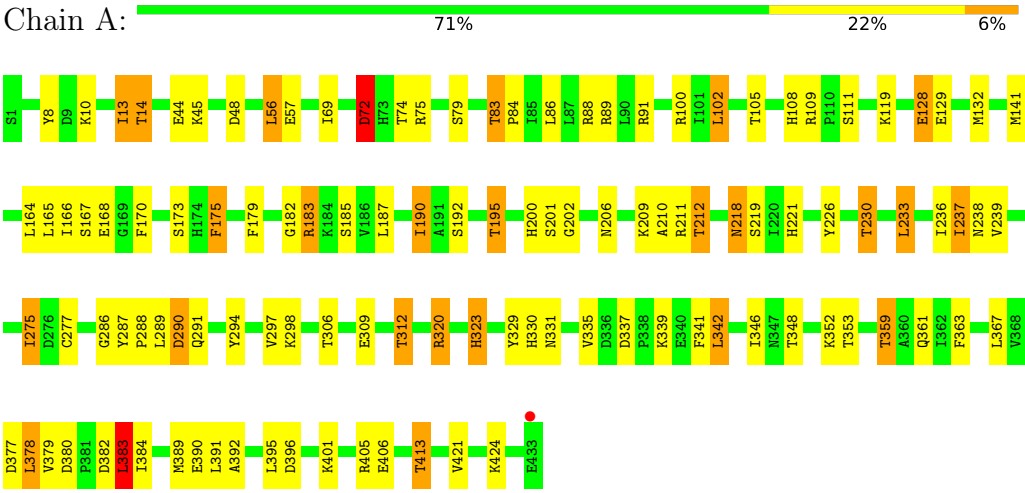
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Ni 1 1	0	0

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.

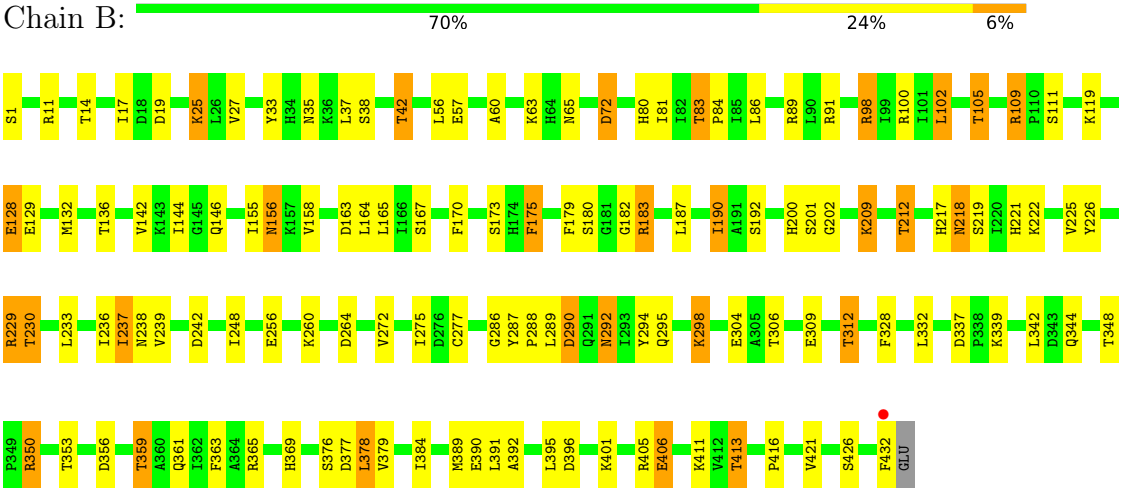
• Molecule 1: Lactate racemization operon protein LarA

Chain A:



• Molecule 1: Lactate racemization operon protein LarA

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	111.28Å 111.28Å 306.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 30.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-3.00) 99.9 (30.00-3.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.88 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.201 , 0.234 0.203 , 0.234	Depositor DCC
R_{free} test set	1953 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	58.1	Xtriage
Anisotropy	0.828	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 22.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6780	wwPDB-VP
Average B, all atoms (Å^2)	68.0	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 4EY, NI

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	0.66	0/3374	0.91	4/4575 (0.1%)
1	B	0.65	0/3370	0.92	4/4570 (0.1%)
All	All	0.65	0/6744	0.92	8/9145 (0.1%)

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	2
1	B	0	2
All	All	0	4

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	383	LEU	CA-CB-CG	6.82	130.99	115.30
1	B	119	LYS	CD-CE-NZ	6.38	126.37	111.70
1	A	383	LEU	CB-CA-C	6.13	121.84	110.20
1	B	405	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	B	109	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	A	72	ASP	CB-CA-C	-5.39	99.61	110.40
1	A	141	MET	CG-SD-CE	-5.20	91.88	100.20
1	B	350	ARG	CG-CD-NE	-5.10	101.09	111.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	289	LEU	Peptide
1	A	290	ASP	Peptide
1	B	289	LEU	Peptide
1	B	290	ASP	Peptide

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	3310	0	3275	95	0
1	B	3306	0	3270	73	0
2	A	24	0	14	2	0
2	B	24	0	12	1	0
3	A	55	0	0	0	0
3	B	60	0	0	3	0
4	B	1	0	0	0	0
All	All	6780	0	6571	169	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 13.

All (169) 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:35:ASN:HD21	1:B:42:THR:HG21	1.08	1.12
1:A:236:ILE:HD12	1:A:255:MET:HA	1.31	1.10
1:A:236:ILE:CD1	1:A:255:MET:HA	1.91	0.99
1:B:226:TYR:O	1:B:230:THR:HG23	1.63	0.96
1:A:363:PHE:CE2	1:A:367:LEU:HD11	2.01	0.94
1:A:183:ARG:HH11	1:A:221:HIS:HD2	1.05	0.94
1:A:226:TYR:O	1:A:230:THR:HG23	1.69	0.93
1:B:35:ASN:ND2	1:B:42:THR:HG21	1.92	0.82
1:A:183:ARG:NH1	1:A:221:HIS:HD2	1.79	0.81
1:A:363:PHE:HE2	1:A:367:LEU:HD11	1.46	0.79
1:B:38:SER:O	1:B:42:THR:HG23	1.83	0.78
1:B:229:ARG:NH1	1:B:256:GLU:OE2	2.18	0.77
1:A:79:SER:O	1:A:83:THR:HG23	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:GLY:H	1:B:238:ASN:HD21	1.33	0.75
1:A:44:GLU:OE1	1:A:89:ARG:NH1	2.21	0.73
1:B:65:ASN:HD21	1:B:100:ARG:HH21	1.36	0.73
1:A:183:ARG:HH11	1:A:221:HIS:CD2	1.98	0.71
1:B:60:ALA:O	1:B:63:LYS:HB2	1.91	0.71
1:A:13:ILE:HD12	1:A:14:THR:N	2.09	0.68
1:A:377:ASP:OD2	1:A:378:LEU:HD12	1.93	0.68
1:A:182:GLY:H	1:A:238:ASN:HD21	1.43	0.67
1:A:56:LEU:HD21	1:A:166:ILE:HD11	1.78	0.66
1:A:218:ASN:C	1:A:218:ASN:HD22	2.00	0.65
1:A:277:CYS:HB3	1:A:413:THR:CG2	2.28	0.64
1:B:226:TYR:CZ	1:B:230:THR:HG21	2.32	0.64
1:B:312:THR:HG23	1:B:406:GLU:OE1	1.96	0.64
1:A:226:TYR:CZ	1:A:230:THR:HG21	2.33	0.63
1:B:277:CYS:HB3	1:B:413:THR:CG2	2.28	0.63
1:A:323:HIS:ND1	1:A:329:TYR:HB2	2.15	0.62
1:A:154:ILE:O	1:A:155:ILE:HD12	2.00	0.62
1:A:75:ARG:O	1:A:119:LYS:NZ	2.33	0.62
1:A:277:CYS:SG	1:A:413:THR:HG23	2.40	0.61
2:B:502:4EY:H1	2:B:502:4EY:H6	1.82	0.61
1:B:260:LYS:HE3	1:B:264:ASP:OD2	2.01	0.61
1:B:91:ARG:NH1	1:B:128:GLU:OE2	2.28	0.61
1:B:37:LEU:HB2	1:B:42:THR:HG22	1.82	0.60
1:A:226:TYR:O	1:A:230:THR:CG2	2.48	0.60
1:A:286:GLY:C	1:A:290:ASP:HB2	2.21	0.60
1:A:376:SER:OG	1:A:379:VAL:HG12	2.02	0.60
1:B:277:CYS:HB3	1:B:413:THR:HG23	1.83	0.60
1:A:277:CYS:HB3	1:A:413:THR:HG23	1.83	0.60
1:A:83:THR:HG22	1:A:168:GLU:OE2	2.02	0.60
1:B:277:CYS:SG	1:B:413:THR:HG23	2.42	0.59
1:A:48:ASP:OD1	1:A:89:ARG:NH2	2.36	0.59
1:A:237:ILE:HD12	1:A:237:ILE:N	2.18	0.59
1:B:179:PHE:O	1:B:183:ARG:NH2	2.33	0.59
1:B:65:ASN:ND2	1:B:100:ARG:HH21	2.01	0.58
1:B:201:SER:HA	1:B:353:THR:HG21	1.84	0.58
1:A:10:LYS:HD2	1:A:320:ARG:NH2	2.17	0.58
1:B:218:ASN:C	1:B:218:ASN:HD22	2.06	0.58
1:A:179:PHE:O	1:A:183:ARG:NH2	2.35	0.58
1:B:102:LEU:HD13	1:B:190:ILE:HG12	1.86	0.58
1:A:297:VAL:HG22	1:A:363:PHE:HD1	1.70	0.57
1:A:233:LEU:HB3	1:A:255:MET:HE2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:TYR:CD2	1:B:248:ILE:HG13	2.40	0.57
1:B:376:SER:OG	1:B:379:VAL:HG12	2.05	0.57
1:A:294:TYR:CZ	1:A:359:THR:HG21	2.40	0.57
1:B:182:GLY:N	1:B:238:ASN:HD21	1.99	0.56
1:B:275:ILE:O	1:B:413:THR:HG21	2.05	0.56
1:A:275:ILE:O	1:A:413:THR:HG21	2.06	0.56
1:B:105:THR:HG23	1:B:132:MET:HE1	1.88	0.56
1:B:390:GLU:OE2	1:B:401:LYS:HD2	2.06	0.55
1:B:237:ILE:HD12	1:B:237:ILE:N	2.22	0.55
1:B:57:GLU:OE2	1:B:89:ARG:HG2	2.05	0.55
1:B:350:ARG:NH2	3:B:508:SO4:O4	2.29	0.55
1:A:331:ASN:HB3	1:A:341:PHE:CE2	2.42	0.55
1:B:226:TYR:O	1:B:230:THR:CG2	2.49	0.55
1:A:182:GLY:N	1:A:238:ASN:HD21	2.04	0.54
1:A:233:LEU:O	1:A:255:MET:HE2	2.06	0.54
1:A:102:LEU:HD13	1:A:190:ILE:HG12	1.89	0.54
1:A:154:ILE:HB	1:A:195:THR:HG21	1.89	0.54
1:A:154:ILE:H	1:A:195:THR:HG21	1.71	0.54
1:B:312:THR:CG2	1:B:406:GLU:OE1	2.56	0.54
1:A:237:ILE:HD12	1:A:237:ILE:H	1.72	0.54
1:B:286:GLY:C	1:B:290:ASP:HB2	2.29	0.54
1:B:298:LYS:NZ	3:B:503:SO4:O4	2.38	0.53
1:A:201:SER:HA	1:A:353:THR:HG21	1.90	0.53
1:B:102:LEU:HD13	1:B:190:ILE:CG1	2.39	0.52
1:B:337:ASP:OD2	1:B:339:LYS:HB3	2.08	0.52
1:A:277:CYS:CB	1:A:413:THR:HG23	2.39	0.52
1:A:91:ARG:NH1	1:A:128:GLU:OE1	2.38	0.52
1:A:236:ILE:HD11	1:A:255:MET:HA	1.85	0.52
1:B:105:THR:CG2	1:B:132:MET:HE1	2.40	0.52
1:B:226:TYR:CE2	1:B:230:THR:HG21	2.44	0.52
1:B:309:GLU:OE2	1:B:369:HIS:ND1	2.38	0.51
1:B:277:CYS:CB	1:B:413:THR:HG23	2.40	0.51
1:A:83:THR:CG2	1:A:168:GLU:OE2	2.59	0.51
1:A:297:VAL:HG22	1:A:363:PHE:CD1	2.46	0.51
1:A:390:GLU:OE2	1:A:401:LYS:HD2	2.11	0.51
1:A:102:LEU:HD13	1:A:190:ILE:CG1	2.41	0.50
1:A:57:GLU:OE2	1:A:89:ARG:HG2	2.11	0.50
1:B:377:ASP:OD2	1:B:378:LEU:HD13	2.12	0.50
1:A:337:ASP:OD2	1:A:339:LYS:HB3	2.12	0.49
1:A:379:VAL:HG11	1:A:384:ILE:HD11	1.94	0.49
1:B:304:GLU:OE2	1:B:365:ARG:NH1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:THR:CG2	1:A:132:MET:HE1	2.43	0.48
1:B:182:GLY:H	1:B:238:ASN:ND2	2.06	0.48
1:B:328:PHE:HB2	1:B:356:ASP:HB3	1.94	0.48
1:A:100:ARG:HG2	1:A:129:GLU:HB3	1.95	0.48
1:A:154:ILE:N	1:A:195:THR:HG21	2.29	0.48
1:B:237:ILE:HD12	1:B:237:ILE:H	1.78	0.48
1:A:183:ARG:NH1	1:A:221:HIS:CD2	2.70	0.48
1:B:287:TYR:CD2	1:B:288:PRO:HA	2.48	0.48
1:A:154:ILE:HB	1:A:195:THR:CG2	2.44	0.48
1:B:72:ASP:OD1	1:B:72:ASP:C	2.52	0.48
1:B:292:ASN:ND2	1:B:295:GLN:H	2.12	0.48
1:A:175:PHE:HA	1:A:212:THR:HB	1.95	0.47
1:A:105:THR:HG23	1:A:132:MET:HE1	1.95	0.47
1:B:83:THR:N	1:B:84:PRO:CD	2.78	0.47
1:A:287:TYR:CD2	1:A:288:PRO:HA	2.50	0.47
1:B:175:PHE:HA	1:B:212:THR:HB	1.97	0.47
1:A:83:THR:N	1:A:84:PRO:CD	2.78	0.47
1:A:202:GLY:HA2	1:A:361:GLN:HE22	1.80	0.46
1:A:391:LEU:HD22	1:A:392:ALA:H	1.80	0.46
1:A:384:ILE:HG23	1:A:389:MET:HB2	1.97	0.46
1:A:391:LEU:HD22	1:A:392:ALA:N	2.30	0.46
1:B:379:VAL:HG11	1:B:384:ILE:HD11	1.98	0.45
1:B:100:ARG:HG2	1:B:129:GLU:HB3	1.97	0.45
1:B:391:LEU:HD22	1:B:392:ALA:N	2.31	0.45
1:A:86:LEU:HD11	1:A:237:ILE:CD1	2.47	0.45
1:B:391:LEU:HD22	1:B:392:ALA:H	1.81	0.45
1:A:72:ASP:HB3	1:A:74:THR:H	1.81	0.45
1:A:363:PHE:CD2	1:A:367:LEU:HD11	2.50	0.45
1:B:63:LYS:HG3	1:B:163:ASP:HB3	2.00	0.44
1:B:202:GLY:HA2	1:B:361:GLN:HE22	1.83	0.44
1:A:69:ILE:HG21	1:A:185:SER:HB3	2.00	0.44
1:A:166:ILE:CG2	1:A:167:SER:N	2.79	0.44
1:B:98:ARG:NH1	1:B:129:GLU:OE2	2.46	0.44
1:A:8:TYR:HB3	1:A:13:ILE:HG23	2.00	0.44
1:B:86:LEU:HD11	1:B:237:ILE:CD1	2.48	0.43
1:A:372:VAL:HG11	1:A:389:MET:CE	2.48	0.43
1:A:108:HIS:CD2	2:A:501:4EY:O2	2.72	0.43
1:A:329:TYR:CE1	1:A:383:LEU:HB2	2.53	0.43
1:A:372:VAL:HG11	1:A:389:MET:HE3	1.99	0.43
1:A:380:ASP:O	1:A:383:LEU:HD22	2.18	0.43
1:A:175:PHE:CE1	1:A:298:LYS:HE3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:GLU:OE2	1:A:369:HIS:ND1	2.44	0.43
1:A:312:THR:HG23	1:A:406:GLU:HG3	2.00	0.43
1:A:377:ASP:OD2	1:A:378:LEU:CD1	2.64	0.43
1:B:294:TYR:CZ	1:B:359:THR:HG21	2.54	0.43
1:B:384:ILE:HG23	1:B:389:MET:HB2	2.00	0.43
1:B:390:GLU:OE2	1:B:401:LYS:CD	2.66	0.43
1:A:384:ILE:HD13	1:A:391:LEU:HD23	2.01	0.43
1:B:80:HIS:CD2	1:B:81:ILE:HG13	2.54	0.43
1:A:75:ARG:CZ	2:A:501:4EY:H11	2.49	0.43
1:A:320:ARG:CB	1:A:320:ARG:HH11	2.32	0.42
1:A:323:HIS:ND1	1:A:329:TYR:CB	2.82	0.42
1:B:332:LEU:CD1	1:B:363:PHE:CD2	3.02	0.42
1:A:44:GLU:OE1	1:A:88:ARG:NH2	2.52	0.42
1:B:221:HIS:CE1	1:B:225:VAL:CG2	3.02	0.42
1:B:344:GLN:O	1:B:348:THR:OG1	2.37	0.42
1:A:74:THR:OG1	1:A:75:ARG:NH1	2.52	0.42
1:A:210:ALA:O	1:A:211:ARG:HG3	2.18	0.42
1:B:167:SER:OG	1:B:236:ILE:HG22	2.19	0.42
1:B:384:ILE:HD13	1:B:391:LEU:HD23	2.02	0.42
1:B:292:ASN:HD22	1:B:295:GLN:H	1.67	0.42
1:A:10:LYS:HD2	1:A:320:ARG:HH21	1.81	0.42
1:B:1:SER:HA	1:B:17:ILE:O	2.19	0.42
1:A:330:HIS:O	1:A:331:ASN:C	2.58	0.41
1:A:342:LEU:HD22	1:A:346:ILE:HD11	2.02	0.41
1:B:209:LYS:HG2	1:B:217:HIS:HB2	2.02	0.41
1:B:25:LYS:HD3	1:B:27:VAL:HG21	2.01	0.41
1:B:426:SER:HB3	3:B:512:SO4:O1	2.20	0.41
1:A:242:ASP:N	1:A:248:ILE:HG12	2.36	0.41
1:B:156:ASN:HD22	1:B:158:VAL:H	1.69	0.41
1:A:83:THR:N	1:A:84:PRO:HD2	2.36	0.41
1:A:275:ILE:HD11	1:A:413:THR:HB	2.03	0.41
1:A:380:ASP:O	1:A:383:LEU:CD2	2.69	0.40
1:A:183:ARG:HD2	1:A:221:HIS:CD2	2.56	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	431/433 (100%)	409 (95%)	21 (5%)	1 (0%)	47 82
1	B	430/433 (99%)	408 (95%)	22 (5%)	0	100 100
All	All	861/866 (99%)	817 (95%)	43 (5%)	1 (0%)	51 85

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	ASP

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	355/360 (99%)	301 (85%)	54 (15%)	3 14
1	B	357/360 (99%)	299 (84%)	58 (16%)	2 12
All	All	712/720 (99%)	600 (84%)	112 (16%)	2 13

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ILE
1	A	14	THR
1	A	45	LYS
1	A	56	LEU
1	A	72	ASP

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Mol	Chain	Res	Type
1	A	83	THR
1	A	102	LEU
1	A	109	ARG
1	A	111	SER
1	A	128	GLU
1	A	144	ILE
1	A	155	ILE
1	A	164	LEU
1	A	165	LEU
1	A	170	PHE
1	A	173	SER
1	A	175	PHE
1	A	183	ARG
1	A	187	LEU
1	A	190	ILE
1	A	192	SER
1	A	195	THR
1	A	200	HIS
1	A	206	ASN
1	A	209	LYS
1	A	212	THR
1	A	218	ASN
1	A	219	SER
1	A	230	THR
1	A	233	LEU
1	A	237	ILE
1	A	239	VAL
1	A	242	ASP
1	A	248	ILE
1	A	275	ILE
1	A	291	GLN
1	A	306	THR
1	A	312	THR
1	A	320	ARG
1	A	323	HIS
1	A	335	VAL
1	A	342	LEU
1	A	348	THR
1	A	352	LYS
1	A	359	THR
1	A	378	LEU
1	A	382	ASP

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Mol	Chain	Res	Type
1	A	383	LEU
1	A	395	LEU
1	A	396	ASP
1	A	405	ARG
1	A	413	THR
1	A	421	VAL
1	A	424	LYS
1	B	11	ARG
1	B	14	THR
1	B	19	ASP
1	B	25	LYS
1	B	42	THR
1	B	56	LEU
1	B	72	ASP
1	B	83	THR
1	B	98	ARG
1	B	102	LEU
1	B	105	THR
1	B	109	ARG
1	B	111	SER
1	B	128	GLU
1	B	136	THR
1	B	142	VAL
1	B	144	ILE
1	B	146	GLN
1	B	155	ILE
1	B	156	ASN
1	B	164	LEU
1	B	165	LEU
1	B	170	PHE
1	B	173	SER
1	B	175	PHE
1	B	180	SER
1	B	183	ARG
1	B	187	LEU
1	B	190	ILE
1	B	192	SER
1	B	200	HIS
1	B	209	LYS
1	B	212	THR
1	B	218	ASN
1	B	219	SER

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Mol	Chain	Res	Type
1	B	222	LYS
1	B	229	ARG
1	B	230	THR
1	B	233	LEU
1	B	237	ILE
1	B	239	VAL
1	B	242	ASP
1	B	272	VAL
1	B	292	ASN
1	B	298	LYS
1	B	306	THR
1	B	312	THR
1	B	342	LEU
1	B	359	THR
1	B	378	LEU
1	B	395	LEU
1	B	396	ASP
1	B	406	GLU
1	B	411	LYS
1	B	413	THR
1	B	416	PRO
1	B	421	VAL
1	B	432	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	HIS
1	A	214	ASN
1	A	218	ASN
1	A	221	HIS
1	A	238	ASN
1	A	259	HIS
1	A	284	ASN
1	A	307	ASN
1	A	357	GLN
1	A	361	GLN
1	B	34	HIS
1	B	35	ASN
1	B	65	ASN
1	B	80	HIS
1	B	156	ASN

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Mol	Chain	Res	Type
1	B	214	ASN
1	B	218	ASN
1	B	238	ASN
1	B	284	ASN
1	B	292	ASN
1	B	307	ASN
1	B	357	GLN
1	B	361	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 26 ligands modelled in this entry, 1 is monoatomic - leaving 25 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	B	508	-	4,4,4	0.48	0	6,6,6	0.46	0
3	SO4	B	505	-	4,4,4	0.44	0	6,6,6	0.57	0
2	4EY	B	502	1,4	22,25,25	1.07	2 (9%)	31,37,37	1.66	9 (29%)
3	SO4	A	508	-	4,4,4	0.49	0	6,6,6	0.30	0
3	SO4	B	511	-	4,4,4	0.41	0	6,6,6	0.19	0
3	SO4	A	507	-	4,4,4	0.40	0	6,6,6	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SO4	B	503	-	4,4,4	0.34	0	6,6,6	0.71	0
3	SO4	A	510	-	4,4,4	0.52	0	6,6,6	0.25	0
3	SO4	B	504	-	4,4,4	0.56	0	6,6,6	0.53	0
3	SO4	A	502	-	4,4,4	0.45	0	6,6,6	0.18	0
3	SO4	B	507	-	4,4,4	0.34	0	6,6,6	0.30	0
3	SO4	B	513	-	4,4,4	0.52	0	6,6,6	0.65	0
3	SO4	A	504	-	4,4,4	0.57	0	6,6,6	0.64	0
3	SO4	B	514	-	4,4,4	0.36	0	6,6,6	0.19	0
3	SO4	A	506	-	4,4,4	0.36	0	6,6,6	0.57	0
3	SO4	A	509	-	4,4,4	0.38	0	6,6,6	0.14	0
3	SO4	A	505	-	4,4,4	0.47	0	6,6,6	0.23	0
3	SO4	B	506	-	4,4,4	0.55	0	6,6,6	0.60	0
3	SO4	B	512	-	4,4,4	0.40	0	6,6,6	0.76	0
2	4EY	A	501	1	22,25,25	1.01	2 (9%)	31,37,37	1.59	5 (16%)
3	SO4	A	511	-	4,4,4	0.44	0	6,6,6	0.79	0
3	SO4	B	510	-	4,4,4	0.54	0	6,6,6	0.44	0
3	SO4	A	512	-	4,4,4	0.62	0	6,6,6	0.37	0
3	SO4	A	503	-	4,4,4	0.44	0	6,6,6	0.48	0
3	SO4	B	509	-	4,4,4	0.41	0	6,6,6	1.07	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	4EY	A	501	1	-	0/12/32/32	0/2/2/2
2	4EY	B	502	1,4	-	8/12/32/32	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	4EY	O4R-C1R	2.86	1.45	1.41
2	A	501	4EY	C2R-C1R	-2.29	1.50	1.53
2	A	501	4EY	O4R-C1R	2.21	1.44	1.41
2	B	502	4EY	C2R-C1R	-2.00	1.50	1.53

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	502	4EY	P-O5R-C5R	4.81	131.55	118.30
2	A	501	4EY	C3-C4-C5	-4.16	117.83	121.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	4EY	O2P-P-O5R	-4.08	95.87	106.73
2	A	501	4EY	O1P-P-O2P	3.20	119.86	107.64
2	B	502	4EY	O5R-P-O3P	-2.51	99.44	106.47
2	B	502	4EY	O1P-P-O5R	2.35	112.98	106.73
2	A	501	4EY	P-O5R-C5R	2.31	124.66	118.30
2	B	502	4EY	O1P-P-O2P	2.31	116.45	107.64
2	B	502	4EY	C5-C6-N1	-2.27	118.20	120.43
2	B	502	4EY	C6-C5-C4	2.20	121.03	118.67
2	A	501	4EY	C6-C5-C4	2.19	121.01	118.67
2	B	502	4EY	O2P-P-O5R	-2.14	101.03	106.73
2	B	502	4EY	C2R-C3R-C4R	2.07	106.67	102.64
2	B	502	4EY	O4R-C1R-C2R	2.02	109.87	106.93

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	502	4EY	C5R-O5R-P-O2P
2	B	502	4EY	C5R-O5R-P-O1P
2	B	502	4EY	O4R-C1R-N1-C2
2	B	502	4EY	O4R-C1R-N1-C6
2	B	502	4EY	O4R-C4R-C5R-O5R
2	B	502	4EY	C5R-O5R-P-O3P
2	B	502	4EY	C3R-C4R-C5R-O5R
2	B	502	4EY	C4R-C5R-O5R-P

There are no ring outliers.

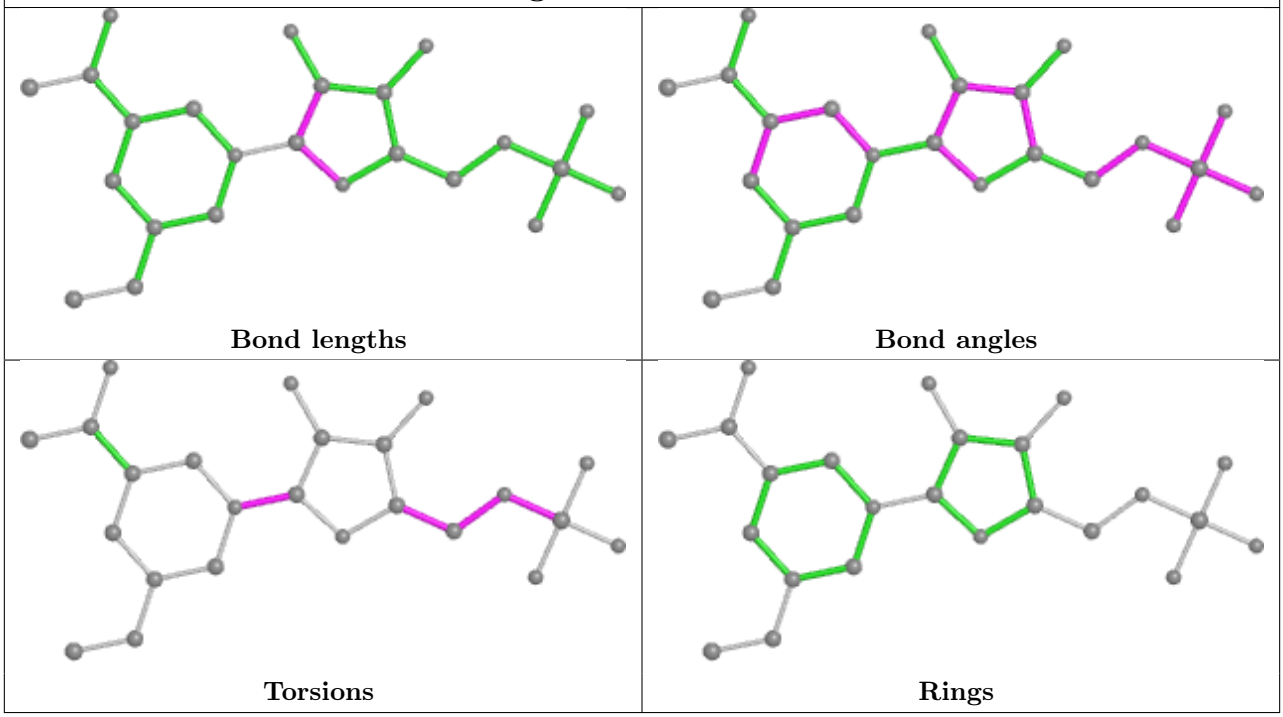
5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	508	SO4	1	0
2	B	502	4EY	1	0
3	B	503	SO4	1	0
3	B	512	SO4	1	0
2	A	501	4EY	2	0

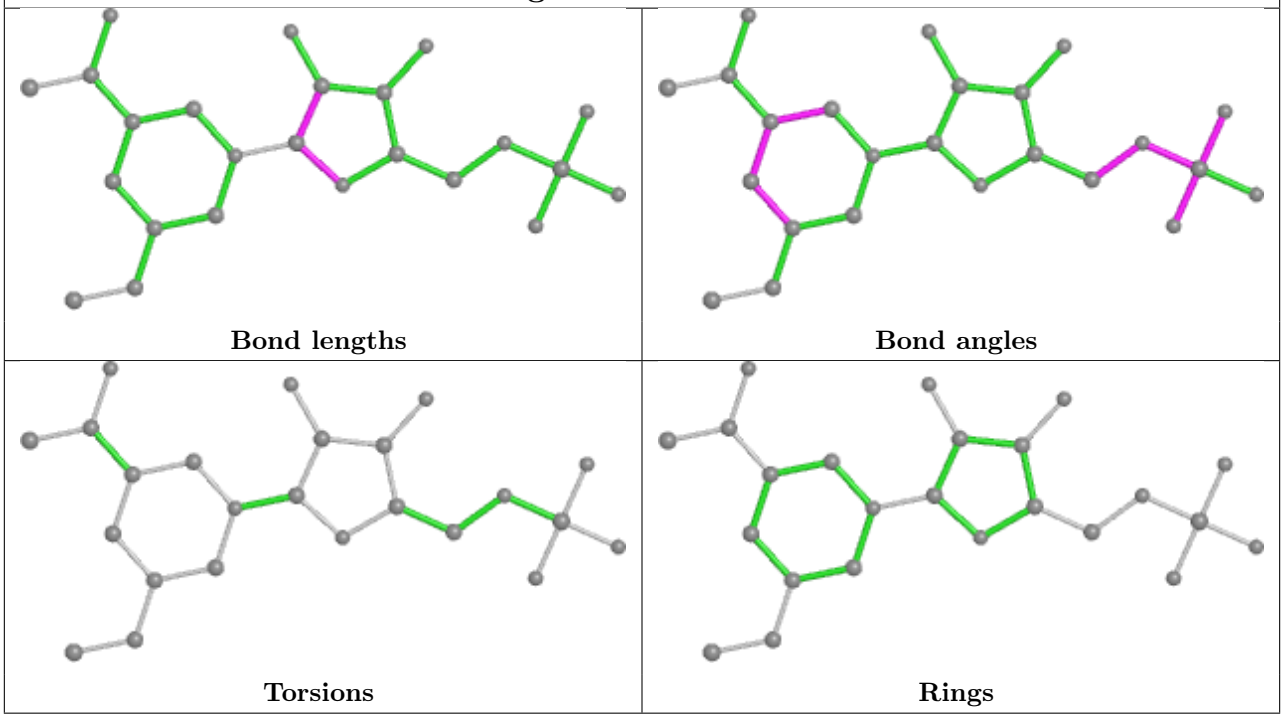
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 4EY B 502



Ligand 4EY A 501



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	433/433 (100%)	-0.44	1 (0%)	95	87	43, 71, 104, 128	0
1	B	432/433 (99%)	-0.65	1 (0%)	95	87	42, 59, 82, 134	0
All	All	865/866 (99%)	-0.55	2 (0%)	95	87	42, 64, 99, 134	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	433	GLU	2.9
1	B	432	PHE	2.2

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides 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. 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
3	SO4	A	507	5/5	0.67	0.41	141,145,162,164	0
3	SO4	B	513	5/5	0.67	0.43	109,120,139,148	0

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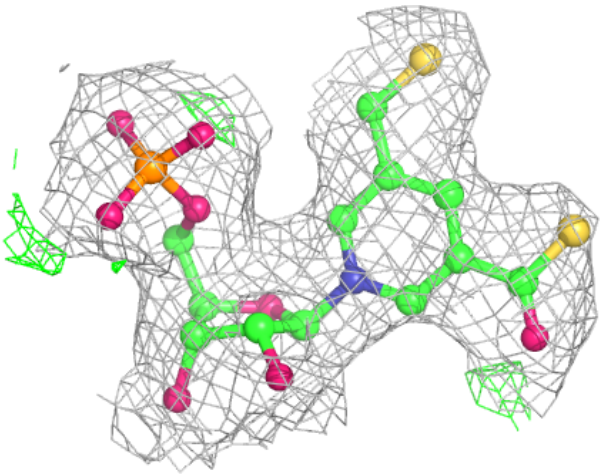
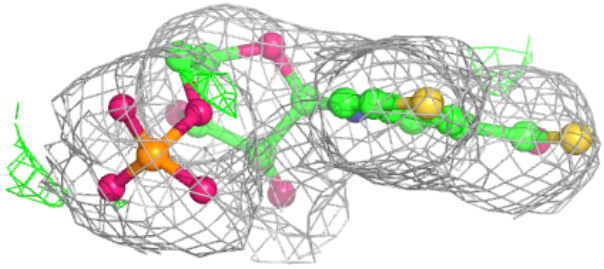
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	A	512	5/5	0.68	0.37	105,112,132,137	0
3	SO4	B	505	5/5	0.73	0.35	87,128,133,154	0
3	SO4	A	505	5/5	0.75	0.48	118,136,143,158	0
3	SO4	B	511	5/5	0.78	0.37	121,138,145,150	0
3	SO4	A	510	5/5	0.85	0.35	114,133,135,138	0
3	SO4	B	506	5/5	0.85	0.25	108,120,125,129	0
3	SO4	B	504	5/5	0.86	0.44	108,118,134,134	0
3	SO4	A	503	5/5	0.87	0.35	101,109,115,127	0
3	SO4	B	510	5/5	0.87	0.44	101,119,135,141	0
3	SO4	A	504	5/5	0.89	0.27	96,98,122,127	0
3	SO4	A	508	5/5	0.91	0.28	97,122,126,133	0
3	SO4	A	509	5/5	0.91	0.24	115,129,144,148	0
3	SO4	B	514	5/5	0.92	0.31	131,134,145,153	0
3	SO4	B	508	5/5	0.93	0.29	98,101,107,116	0
3	SO4	B	507	5/5	0.94	0.31	99,102,107,122	0
3	SO4	A	502	5/5	0.94	0.18	85,99,105,108	0
3	SO4	A	506	5/5	0.95	0.36	96,97,102,103	0
2	4EY	A	501	24/24	0.96	0.19	45,58,68,101	0
3	SO4	A	511	5/5	0.96	0.14	70,79,84,92	0
3	SO4	B	509	5/5	0.97	0.17	71,75,82,89	0
3	SO4	B	512	5/5	0.97	0.12	52,63,70,76	0
3	SO4	B	503	5/5	0.98	0.16	75,82,91,110	0
2	4EY	B	502	24/24	0.98	0.20	45,50,65,72	0
4	NI	B	501	1/1	0.99	0.14	64,64,64,64	0

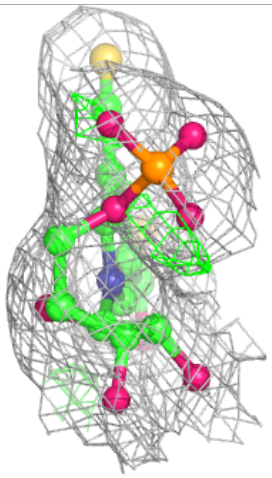
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 4EY A 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

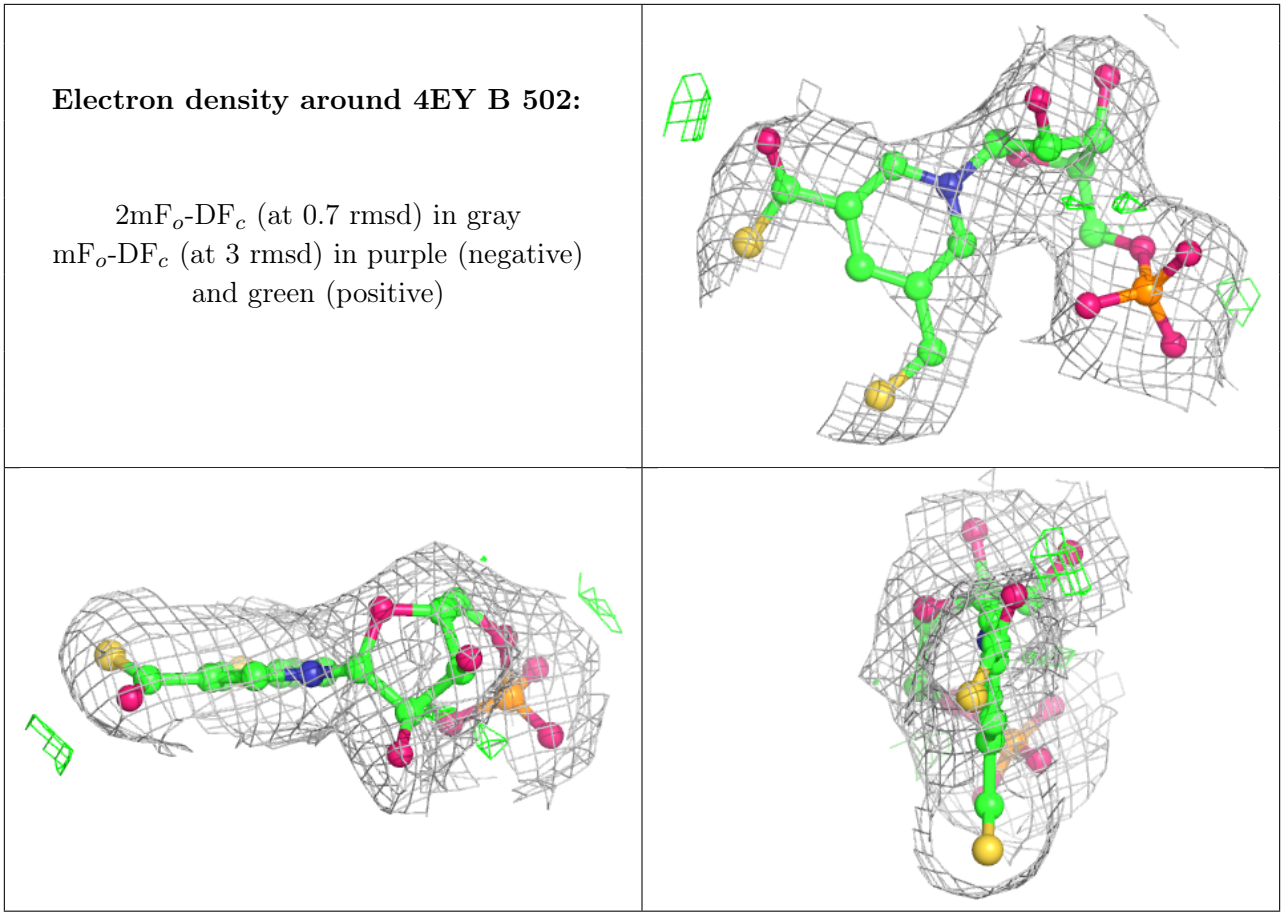






Electron density around 4EY B 502:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.