Full wwPDB X-ray Structure Validation Report (i)

Sep 25, 2023 – 07:14 PM EDT

PDB ID	:	5WLW
Title	:	Crystal Structure of the Human Mitochondrial Cysteine Desulfurase with active Cysteine Loop within ISCU1 active site, coordinating Zn ion. Complexed with human ISD11 and E. coli ACP1 at 3.3A.
Authors	:	Boniecki, M.T.; Cygler, M.
Deposited on	:	2017-07-27
Resolution	:	3.32 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 (i) 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 (i)) were used in the production of this report:

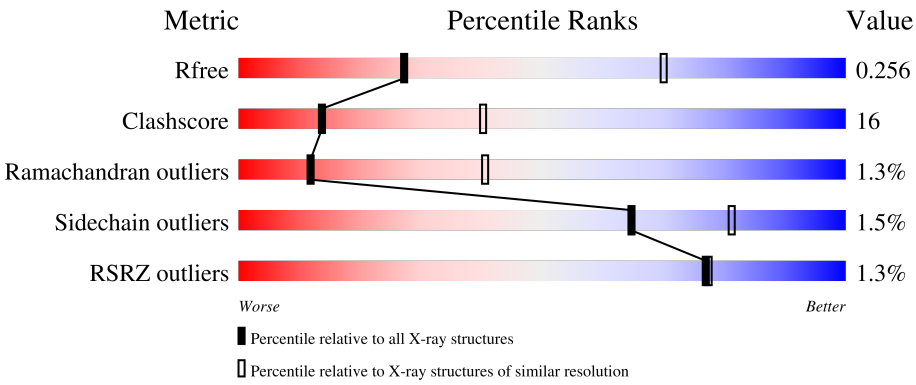
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.32 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	1089 (3.36-3.28)
Clashscore	141614	1137 (3.36-3.28)
Ramachandran outliers	138981	1115 (3.36-3.28)
Sidechain outliers	138945	1114 (3.36-3.28)
RSRZ outliers	127900	1059 (3.36-3.28)

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	406	71% 27% • •
1	E	406	72% 26% • •
2	B	91	% 70% 18% • 11%
2	F	91	66% 24% • 9%

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Mol	Chain	Length	Quality of chain
3	C	77	5% 65% 25% • 8%
3	G	77	3% 66% 22% • 9%
4	D	150	7% 56% 29% • 15%
4	H	150	51% 29% • 17%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 9866 atoms, of which 1 is hydrogen 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 Cysteine desulfurase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	399	2936	1855	504	557	20	0	0	0
1	E	401	2954	1863	513	558	20	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	52	MET	-	initiating methionine	UNP Q9Y697
A	53	GLY	-	expression tag	UNP Q9Y697
A	54	SER	-	expression tag	UNP Q9Y697
A	55	SER	-	expression tag	UNP Q9Y697
E	52	MET	-	initiating methionine	UNP Q9Y697
E	53	GLY	-	expression tag	UNP Q9Y697
E	54	SER	-	expression tag	UNP Q9Y697
E	55	SER	-	expression tag	UNP Q9Y697

- Molecule 2 is a protein called LYR motif-containing protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	81	633	400	120	112	1	0	0	0
2	F	83	645	410	120	114	1	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	11	ALA	SER	variant	UNP Q9HD34
F	11	ALA	SER	variant	UNP Q9HD34

- Molecule 3 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	71	439	276	73	89	1	0	0	0
3	G	70	468	296	74	97	1	0	0	0

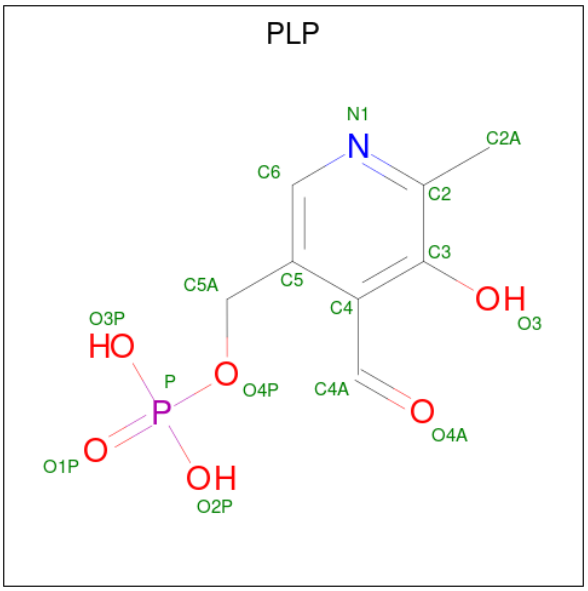
- Molecule 4 is a protein called Iron-sulfur cluster assembly enzyme ISCU, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	128	820	514	143	158	5	0	0	0
4	H	124	870	548	147	170	5	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

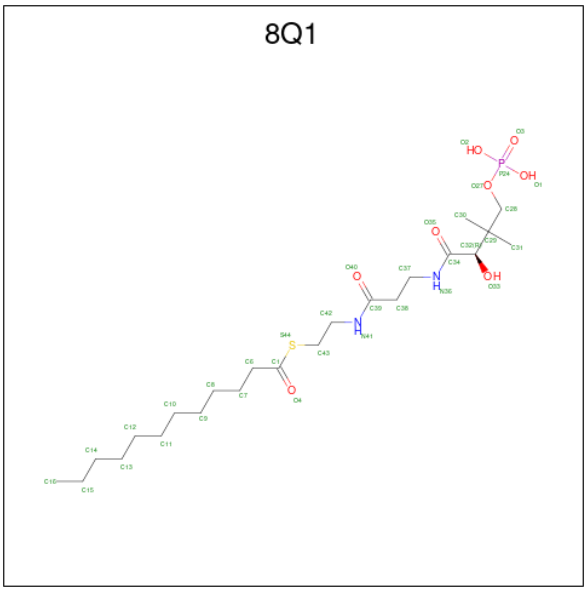
Chain	Residue	Modelled	Actual	Comment	Reference
D	115	ILE	MET	engineered mutation	UNP Q9H1K1
D	143	GLU	-	expression tag	UNP Q9H1K1
D	144	LEU	-	expression tag	UNP Q9H1K1
D	145	HIS	-	expression tag	UNP Q9H1K1
D	146	HIS	-	expression tag	UNP Q9H1K1
D	147	HIS	-	expression tag	UNP Q9H1K1
D	148	HIS	-	expression tag	UNP Q9H1K1
D	149	HIS	-	expression tag	UNP Q9H1K1
D	150	HIS	-	expression tag	UNP Q9H1K1
H	115	ILE	MET	engineered mutation	UNP Q9H1K1
H	143	GLU	-	expression tag	UNP Q9H1K1
H	144	LEU	-	expression tag	UNP Q9H1K1
H	145	HIS	-	expression tag	UNP Q9H1K1
H	146	HIS	-	expression tag	UNP Q9H1K1
H	147	HIS	-	expression tag	UNP Q9H1K1
H	148	HIS	-	expression tag	UNP Q9H1K1
H	149	HIS	-	expression tag	UNP Q9H1K1
H	150	HIS	-	expression tag	UNP Q9H1K1

- Molecule 5 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P 15 8 1 5 1	0	0
5	E	1	Total C H N O P 16 8 1 1 5 1	0	0

- Molecule 6 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C N O P S 34 23 2 7 1 1	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
6	G	1	34	23	2	7	1	1	0	0

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
7	D	1	1	1	0	0
			Total	Zn		
7	H	1	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: Cysteine desulfurase, mitochondrial

Chain A:

• Molecule 1: Cysteine desulfurase, mitochondrial

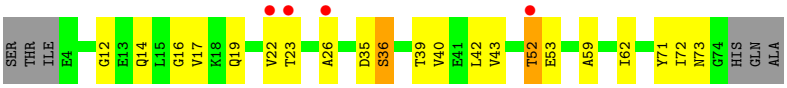
Chain E:

• Molecule 2: LYR motif-containing protein 4

Chain B:

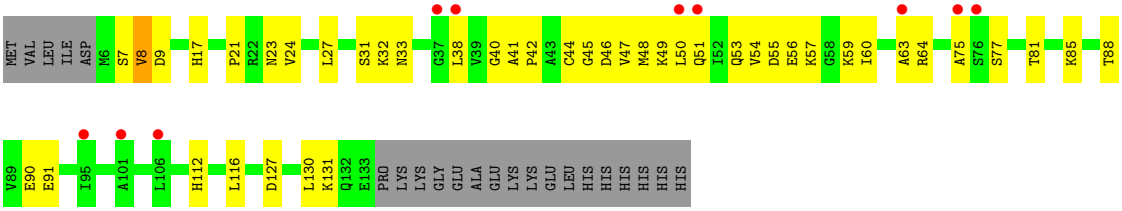
• Molecule 2: LYR motif-containing protein 4

• Molecule 3: Acyl carrier protein

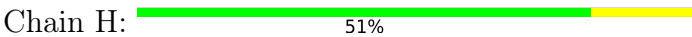


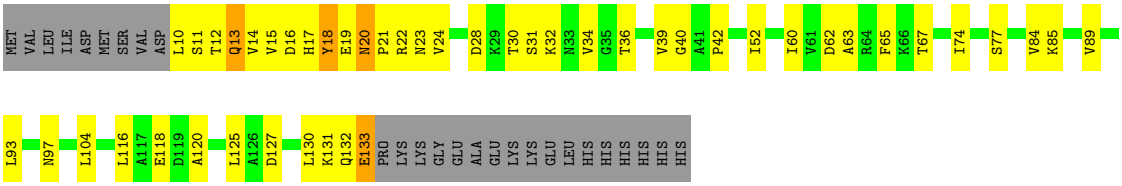
• Molecule 3: Acyl carrier protein

• Molecule 4: Iron-sulfur cluster assembly enzyme ISCU, mitochondrial



• Molecule 4: Iron-sulfur cluster assembly enzyme ISCU, mitochondrial





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	97.53Å 121.24Å 151.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.76 – 3.32 48.76 – 3.32	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.76-3.32) 99.8 (48.76-3.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.196 , 0.255 0.198 , 0.256	Depositor DCC
R_{free} test set	2000 reflections (7.35%)	wwPDB-VP
Wilson B-factor (Å^2)	78.9	Xtriage
Anisotropy	0.795	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 57.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9866	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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: PLP, 8Q1, ZN

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	0.27	0/2991	0.45	0/4070
1	E	0.27	0/3009	0.45	0/4093
2	B	0.25	0/641	0.42	0/867
2	F	0.25	0/653	0.40	0/883
3	C	0.24	0/441	0.45	0/608
3	G	0.25	0/471	0.46	0/647
4	D	0.24	0/831	0.43	0/1142
4	H	0.45	0/881	0.52	0/1201
All	All	0.28	0/9918	0.45	0/13511

There are no bond length outliers.

There are no bond angle outliers.

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	2936	0	2804	83	0
1	E	2954	0	2822	83	0
2	B	633	0	607	14	0
2	F	645	0	630	21	0
3	C	439	0	348	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	468	0	394	17	0
4	D	820	0	691	37	0
4	H	870	0	845	52	0
5	A	15	0	7	2	0
5	E	15	1	7	2	0
6	C	34	0	0	2	0
6	G	34	0	0	4	0
7	D	1	0	0	0	0
7	H	1	0	0	0	0
All	All	9865	1	9155	302	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 16.

All (302) 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)
4:H:20:ASN:H	4:H:21:PRO:CD	1.54	1.15
2:F:6:ARG:NH2	6:G:301:8Q1:O3	1.83	1.12
1:A:122:ILE:HD12	1:A:270:ILE:HD12	1.38	1.03
4:H:20:ASN:H	4:H:21:PRO:HD3	1.23	0.99
1:A:117:ASP:OD1	1:A:118:PRO:HD2	1.63	0.98
1:A:271:ARG:HD3	1:A:274:PRO:HD2	1.45	0.98
4:H:20:ASN:N	4:H:21:PRO:CD	2.21	0.97
4:H:20:ASN:O	4:H:22:ARG:NE	2.01	0.94
3:G:59:ALA:HA	3:G:62:ILE:HD13	1.48	0.93
3:C:59:ALA:HA	3:C:62:ILE:HD13	1.52	0.92
1:A:127:ALA:HB2	1:A:255:SER:HB2	1.55	0.89
4:H:16:ASP:O	4:H:20:ASN:HB2	1.73	0.88
1:A:321:ARG:NH2	1:A:414:THR:O	2.06	0.87
1:A:442:MET:O	1:A:446:GLY:N	2.09	0.85
1:E:321:ARG:NH2	1:E:414:THR:O	2.08	0.85
1:A:337:LEU:HD11	1:A:427:ILE:HA	1.58	0.83
4:D:38:LEU:HD13	4:D:49:LYS:HB2	1.62	0.82
1:E:438:PRO:O	1:E:442:MET:HG3	1.82	0.79
1:A:392:LEU:O	1:A:397:THR:HG22	1.84	0.78
2:B:41:ARG:NH1	3:C:35:ASP:OD2	2.17	0.77
1:E:228:TYR:CE2	1:E:276:VAL:HG13	2.20	0.76
4:H:19:GLU:HA	4:H:21:PRO:HD3	1.66	0.75
4:H:20:ASN:N	4:H:21:PRO:HD3	1.93	0.75
1:E:366:LEU:O	1:E:370:LEU:HD12	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:12:GLY:O	3:C:16:GLY:N	2.20	0.74
4:D:8:VAL:HG13	4:D:9:ASP:H	1.50	0.74
1:E:298:THR:HB	1:E:299:PRO:HD3	1.70	0.72
2:B:55:LEU:HB3	6:C:301:8Q1:O4	1.88	0.72
6:C:301:8Q1:O40	6:C:301:8Q1:N36	2.21	0.72
1:E:136:LYS:HB2	1:E:281:LEU:HD11	1.71	0.72
1:A:107:ARG:NH2	1:A:121:ILE:O	2.23	0.72
1:A:366:LEU:O	1:A:370:LEU:HD12	1.91	0.70
4:H:65:PHE:CD1	4:H:67:THR:HG23	2.27	0.70
1:A:438:PRO:O	1:A:442:MET:HG3	1.93	0.69
4:D:60:ILE:HB	4:D:85:LYS:O	1.90	0.69
4:D:130:LEU:HD13	4:D:130:LEU:O	1.93	0.69
4:H:89:VAL:HG13	4:H:125:LEU:HD22	1.74	0.68
1:A:117:ASP:OD1	1:A:118:PRO:CD	2.39	0.68
1:E:135:ILE:HD11	1:E:159:VAL:HG13	1.76	0.68
4:D:27:LEU:N	4:D:51:GLN:OE1	2.20	0.68
1:A:122:ILE:CD1	1:A:270:ILE:HD12	2.20	0.68
1:A:122:ILE:HD12	1:A:270:ILE:CD1	2.20	0.67
1:A:258:LYS:NZ	5:A:501:PLP:O3	2.26	0.67
1:A:260:TYR:OH	1:A:412:ARG:N	2.22	0.67
1:A:317:TYR:OH	2:B:38:ASP:OD2	2.10	0.67
1:A:326:SER:OG	1:A:354:ILE:HD11	1.95	0.67
2:B:81:LEU:N	2:B:84:GLU:OE1	2.24	0.66
1:E:449:LEU:H	1:E:449:LEU:HD22	1.61	0.66
1:A:392:LEU:HB3	1:A:397:THR:HG21	1.77	0.65
3:G:59:ALA:HA	3:G:62:ILE:CD1	2.27	0.64
1:A:441:GLU:OE1	4:D:49:LYS:NZ	2.29	0.64
1:A:135:ILE:HD11	1:A:159:VAL:HG13	1.80	0.64
1:E:94:ALA:O	1:E:98:GLU:HG2	1.97	0.64
1:E:120:GLU:CG	1:E:272:ARG:HG2	2.28	0.64
1:E:120:GLU:OE1	1:E:271:ARG:HA	1.98	0.64
1:A:273:ARG:CB	1:A:274:PRO:CD	2.76	0.63
2:B:62:ASP:O	2:B:65:VAL:HG12	1.99	0.63
1:E:321:ARG:HH21	1:E:325:LEU:HD11	1.62	0.63
4:D:46:ASP:OD2	4:D:112:HIS:NE2	2.31	0.63
1:E:273:ARG:CB	1:E:274:PRO:CD	2.77	0.63
4:H:36:THR:HG22	4:H:127:ASP:OD2	1.98	0.63
1:E:127:ALA:HB2	1:E:255:SER:HB2	1.81	0.63
1:E:326:SER:OG	1:E:354:ILE:HD11	1.98	0.62
1:A:362:GLU:OE1	1:A:364:GLU:N	2.33	0.62
1:E:111:ALA:N	1:E:121:ILE:HD11	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:6:ARG:CZ	6:G:301:8Q1:O3	2.48	0.62
4:D:127:ASP:O	4:D:131:LYS:HG2	1.99	0.62
1:A:136:LYS:O	1:A:140:ARG:HG3	2.00	0.61
1:A:237:VAL:HG21	1:A:254:ILE:HG12	1.82	0.61
4:H:65:PHE:HD1	4:H:67:THR:HG23	1.63	0.61
1:A:374:ALA:HB1	1:E:93:HIS:CG	2.36	0.61
4:D:23:ASN:O	4:D:64:ARG:HA	2.01	0.61
3:G:7:VAL:HG12	3:G:50:PHE:CZ	2.36	0.61
1:A:241:PRO:O	1:A:242:LEU:HD23	2.01	0.60
1:E:365:SER:O	4:H:18:TYR:OH	2.18	0.60
1:A:265:VAL:HB	1:A:300:LEU:HB3	1.81	0.60
4:D:17:HIS:HB2	4:D:75:ALA:HB1	1.83	0.60
4:H:12:THR:HG23	4:H:13:GLN:OE1	2.01	0.60
4:H:52:ILE:HD11	4:H:125:LEU:HD23	1.84	0.60
4:H:67:THR:OG1	4:H:74:ILE:HD13	2.01	0.60
4:D:23:ASN:HB3	4:D:63:ALA:O	2.02	0.59
1:E:110:VAL:HB	1:E:121:ILE:HD13	1.83	0.59
1:E:136:LYS:O	1:E:140:ARG:HG3	2.02	0.59
1:A:135:ILE:CD1	1:A:159:VAL:HG13	2.33	0.59
4:D:21:PRO:HB2	4:D:24:VAL:HG21	1.84	0.59
1:E:111:ALA:CA	1:E:121:ILE:HD11	2.32	0.59
2:F:48:ASP:OD1	2:F:50:VAL:HG12	2.03	0.59
1:E:258:LYS:NZ	5:E:501:PLP:O3	2.34	0.59
3:C:23:THR:OG1	3:C:26:ALA:HB2	2.03	0.58
3:G:58:GLU:O	3:G:61:LYS:HG2	2.04	0.58
4:D:8:VAL:HG13	4:D:9:ASP:N	2.18	0.58
1:A:342:MET:HA	1:A:356:LEU:HD23	1.85	0.58
4:H:130:LEU:O	4:H:130:LEU:HD13	2.03	0.58
1:E:189:LEU:O	1:E:193:ILE:HG13	2.04	0.57
4:H:16:ASP:O	4:H:20:ASN:CB	2.49	0.57
1:E:148:HIS:C	1:E:149:LEU:HD12	2.24	0.57
1:E:94:ALA:HA	1:E:97:TRP:CE3	2.39	0.57
3:C:36:SER:O	3:C:39:THR:OG1	2.15	0.57
4:H:52:ILE:CD1	4:H:125:LEU:HD23	2.35	0.57
3:G:35:ASP:O	3:G:39:THR:HG23	2.04	0.57
4:D:44:CYS:O	4:D:46:ASP:N	2.38	0.57
1:E:86:GLY:HA3	1:E:95:TYR:HB3	1.87	0.56
1:A:127:ALA:CB	1:A:255:SER:HB2	2.33	0.56
4:D:21:PRO:HB2	4:D:24:VAL:CG2	2.35	0.56
1:E:278:VAL:HB	1:E:291:MET:CE	2.35	0.56
3:C:35:ASP:O	3:C:39:THR:HG23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:52:ILE:HD12	4:H:60:ILE:CD1	2.36	0.56
1:A:381:CYS:SG	4:D:44:CYS:HB3	2.46	0.56
1:A:277:ARG:HE	1:A:277:ARG:HA	1.69	0.56
4:H:17:HIS:O	4:H:18:TYR:O	2.24	0.56
1:E:318:ASP:OD2	1:E:412:ARG:HD3	2.06	0.55
1:A:357:SER:HA	1:A:404:SER:O	2.05	0.55
4:H:67:THR:HG21	4:H:77:SER:OG	2.07	0.55
1:A:284:GLY:HA2	1:E:158:CYS:HA	1.88	0.55
4:D:88:THR:HG22	4:D:90:GLU:H	1.71	0.55
4:H:31:SER:O	4:H:131:LYS:HE2	2.07	0.54
1:E:151:THR:OG1	1:E:155:GLU:HG3	2.08	0.54
1:A:298:THR:HB	1:A:299:PRO:HD3	1.89	0.54
4:D:8:VAL:HG22	4:D:9:ASP:N	2.22	0.54
4:H:93:LEU:CD1	4:H:125:LEU:HD13	2.38	0.54
3:C:19:GLN:O	3:C:22:VAL:HG22	2.08	0.53
4:D:31:SER:C	4:D:33:ASN:H	2.12	0.53
4:H:32:LYS:HA	4:H:131:LYS:HE3	1.90	0.53
4:H:39:VAL:HG22	4:H:116:LEU:HD11	1.90	0.53
2:F:13:TYR:OH	3:G:41:GLU:OE2	2.24	0.53
1:E:228:TYR:HE2	1:E:276:VAL:HG13	1.73	0.53
1:E:217:GLU:HA	1:E:217:GLU:OE1	2.08	0.53
2:F:44:LYS:O	6:G:301:8Q1:C37	2.57	0.53
4:D:41:ALA:N	4:D:46:ASP:O	2.32	0.52
3:G:20:GLU:N	3:G:20:GLU:OE2	2.42	0.52
1:E:453:LYS:HA	4:H:40:GLY:O	2.10	0.52
4:H:20:ASN:N	4:H:21:PRO:HD2	2.21	0.52
1:E:251:LEU:HA	1:E:269:TYR:O	2.10	0.52
2:F:23:PHE:CG	2:F:70:VAL:HG22	2.45	0.52
1:A:297:PRO:CB	1:A:300:LEU:HD12	2.40	0.52
1:A:350:TYR:CE2	1:A:352:GLY:HA3	2.45	0.52
2:F:17:LEU:O	2:F:21:LYS:HG3	2.09	0.52
1:E:442:MET:O	1:E:446:GLY:N	2.42	0.51
4:D:40:GLY:HA2	4:D:47:VAL:HA	1.91	0.51
1:A:63:VAL:HG22	1:A:409:GLY:HA3	1.92	0.51
2:B:66:ILE:O	2:B:70:VAL:HG23	2.11	0.51
1:A:334:MET:SD	1:A:340:VAL:HG13	2.50	0.51
1:E:111:ALA:N	1:E:121:ILE:CD1	2.74	0.50
1:A:181:SER:HB2	1:A:345:ASP:HB2	1.93	0.50
1:E:273:ARG:O	1:E:275:ARG:N	2.43	0.50
3:C:71:TYR:C	3:C:73:ASN:H	2.15	0.50
4:D:50:LEU:HD12	4:D:64:ARG:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:54:VAL:HG13	4:D:59:LYS:O	2.12	0.50
1:E:449:LEU:HD22	1:E:449:LEU:N	2.27	0.50
2:F:6:ARG:NH2	3:G:36:SER:HB3	2.26	0.50
1:E:181:SER:HB2	1:E:345:ASP:HB2	1.94	0.49
3:C:52:THR:HG23	3:C:53:GLU:N	2.27	0.49
1:E:265:VAL:HB	1:E:300:LEU:HB3	1.94	0.49
1:A:204:THR:HA	1:A:215:ILE:HD11	1.94	0.49
1:E:278:VAL:HB	1:E:291:MET:HE1	1.95	0.49
2:F:34:ARG:CZ	2:F:34:ARG:HB3	2.42	0.49
1:A:57:ARG:NH1	1:E:98:GLU:OE1	2.40	0.49
1:E:406:ILE:HD11	1:E:408:PHE:CZ	2.47	0.49
1:E:59:LEU:HD22	1:E:418:GLU:HG2	1.93	0.49
1:E:103:MET:SD	1:E:296:VAL:HG11	2.53	0.49
1:E:350:TYR:CE2	1:E:352:GLY:HA3	2.48	0.48
1:A:83:ASN:ND2	2:F:76:TYR:O	2.45	0.48
1:A:297:PRO:HB2	1:A:300:LEU:HD12	1.94	0.48
1:A:380:ALA:O	1:A:382:THR:N	2.41	0.48
1:A:75:ASP:CG	2:B:65:VAL:HG23	2.34	0.48
1:E:135:ILE:CD1	1:E:159:VAL:HG13	2.41	0.48
4:H:84:VAL:HG12	4:H:84:VAL:O	2.13	0.48
1:A:426:CYS:O	1:A:430:VAL:HG23	2.13	0.48
1:E:228:TYR:CD2	1:E:276:VAL:HG13	2.48	0.48
1:E:377:SER:OG	1:E:405:SER:O	2.16	0.48
1:A:273:ARG:CB	1:A:274:PRO:HD3	2.44	0.48
1:A:342:MET:HA	1:A:356:LEU:CD2	2.43	0.48
1:E:320:LYS:O	1:E:323:SER:OG	2.31	0.48
4:D:38:LEU:CD1	4:D:49:LYS:HB2	2.41	0.48
2:F:16:MET:O	2:F:20:SER:OG	2.14	0.48
3:G:27:SER:O	3:G:31:ASP:HB2	2.14	0.47
1:A:158:CYS:HA	1:E:284:GLY:HA2	1.96	0.47
1:E:436:MET:HG2	4:H:24:VAL:HG11	1.96	0.47
2:B:80:LYS:HB3	2:B:84:GLU:OE1	2.14	0.47
1:E:372:ASP:HB3	2:F:82:ILE:HD13	1.96	0.47
4:H:10:LEU:CD2	4:H:15:VAL:HG23	2.44	0.47
4:D:54:VAL:HG12	4:D:55:ASP:O	2.15	0.47
2:F:27:ASN:OD1	2:F:27:ASN:N	2.47	0.47
5:A:501:PLP:O3P	1:E:295:THR:HB	2.14	0.47
3:G:63:THR:O	3:G:63:THR:HG22	2.15	0.47
1:E:419:VAL:O	1:E:423:VAL:HG23	2.14	0.47
1:A:356:LEU:O	1:A:405:SER:HA	2.15	0.47
1:E:377:SER:HB2	1:E:406:ILE:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:39:VAL:HG22	4:H:116:LEU:CD1	2.45	0.47
1:A:295:THR:OG1	5:E:501:PLP:O3P	2.24	0.46
4:H:127:ASP:O	4:H:131:LYS:HG3	2.15	0.46
3:C:14:GLN:CB	3:C:42:LEU:HD13	2.45	0.46
1:E:228:TYR:CE2	1:E:276:VAL:HG22	2.51	0.46
4:H:39:VAL:CG1	4:H:120:ALA:HB2	2.45	0.46
1:E:111:ALA:HB1	1:E:116:ALA:O	2.16	0.46
1:A:352:GLY:O	1:A:409:GLY:HA2	2.15	0.46
1:E:64:GLN:NE2	1:E:353:CYS:HB2	2.30	0.46
1:A:86:GLY:HA3	1:A:95:TYR:HB3	1.98	0.46
4:H:19:GLU:CA	4:H:21:PRO:HD3	2.41	0.46
1:E:366:LEU:CD1	1:E:370:LEU:HD11	2.46	0.46
1:E:397:THR:HG22	1:E:398:ASP:O	2.16	0.46
4:D:48:MET:SD	4:D:77:SER:OG	2.72	0.46
1:A:106:ALA:HA	1:A:109:GLN:OE1	2.16	0.45
1:A:178:VAL:HG12	1:A:184:ILE:HG22	1.98	0.45
4:D:27:LEU:HD13	4:D:53:GLN:HB2	1.97	0.45
1:A:251:LEU:HA	1:A:269:TYR:O	2.15	0.45
2:F:48:ASP:HB3	2:F:51:GLU:CG	2.46	0.45
1:A:350:TYR:CD1	1:A:351:PRO:HD2	2.52	0.45
1:E:306:ALA:O	1:E:310:VAL:HG23	2.16	0.45
4:H:21:PRO:HG2	4:H:21:PRO:O	2.16	0.45
1:A:129:GLU:O	1:A:133:ILE:HG13	2.16	0.45
1:E:90:SER:O	1:E:96:GLY:HA3	2.15	0.45
4:H:11:SER:OG	4:H:14:VAL:HG23	2.16	0.45
3:G:44:MET:HE2	3:G:44:MET:HB3	1.87	0.45
4:H:10:LEU:HD23	4:H:11:SER:O	2.17	0.45
4:H:93:LEU:HD12	4:H:125:LEU:HD13	1.99	0.45
1:E:342:MET:HA	1:E:356:LEU:HD23	1.98	0.45
3:G:42:LEU:C	3:G:42:LEU:HD23	2.38	0.45
4:H:10:LEU:HD23	4:H:10:LEU:C	2.37	0.44
4:H:93:LEU:HD12	4:H:125:LEU:CD1	2.47	0.44
1:A:73:VAL:O	1:A:77:MET:HG3	2.17	0.44
4:D:88:THR:HB	4:D:91:GLU:H	1.83	0.44
1:E:426:CYS:O	1:E:430:VAL:HG23	2.18	0.44
1:E:278:VAL:HB	1:E:291:MET:HE3	1.99	0.44
3:G:72:ILE:O	3:G:72:ILE:HG22	2.17	0.44
1:E:63:VAL:HG22	1:E:409:GLY:HA3	2.00	0.44
2:F:12:LEU:HD12	2:F:12:LEU:HA	1.82	0.44
4:D:23:ASN:HB2	4:D:81:THR:OG1	2.18	0.44
1:E:278:VAL:O	1:E:291:MET:HE1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:131:LYS:HB2	4:H:132:GLN:HE21	1.82	0.43
2:B:68:ARG:HG2	2:F:75:LEU:HD22	1.99	0.43
4:D:46:ASP:OD2	4:D:112:HIS:CD2	2.71	0.43
4:H:11:SER:OG	4:H:13:GLN:HG2	2.18	0.43
2:B:68:ARG:O	2:B:72:ILE:HG12	2.19	0.43
3:C:12:GLY:HA2	3:C:17:VAL:HG12	2.01	0.43
1:E:273:ARG:CB	1:E:274:PRO:HD2	2.49	0.43
4:D:31:SER:O	4:D:33:ASN:N	2.49	0.43
2:B:25:ALA:HB1	2:B:27:ASN:OD1	2.18	0.43
4:D:41:ALA:HB2	4:D:116:LEU:HD22	2.00	0.43
3:C:14:GLN:HG2	3:C:42:LEU:HA	2.00	0.43
1:E:345:ASP:O	1:E:349:HIS:HB2	2.18	0.43
2:F:57:ASN:O	2:F:61:ARG:HG3	2.19	0.43
4:H:133:GLU:OE2	4:H:133:GLU:HA	2.19	0.43
1:A:150:ILE:HD11	1:A:193:ILE:HA	2.01	0.42
1:A:282:GLN:NE2	1:A:293:SER:O	2.48	0.42
1:E:413:PHE:HB3	2:F:27:ASN:HB2	2.01	0.42
1:E:357:SER:HA	1:E:404:SER:O	2.19	0.42
4:H:28:ASP:OD1	4:H:30:THR:OG1	2.32	0.42
1:A:70:ASP:O	1:A:73:VAL:N	2.52	0.42
1:A:120:GLU:OE1	1:A:269:TYR:HE1	2.03	0.42
2:B:23:PHE:O	2:B:29:ARG:NH1	2.50	0.42
3:C:40:VAL:O	3:C:43:VAL:HG22	2.19	0.42
1:A:380:ALA:C	1:A:382:THR:H	2.22	0.42
1:A:106:ALA:O	1:A:109:GLN:HB2	2.20	0.42
3:C:62:ILE:HD12	3:C:62:ILE:N	2.34	0.42
4:D:56:GLU:O	4:D:57:LYS:CB	2.67	0.42
1:A:70:ASP:OD2	1:A:412:ARG:NH2	2.48	0.42
2:B:12:LEU:HD12	2:B:12:LEU:HA	1.65	0.42
1:E:147:LYS:HE2	1:E:147:LYS:HB3	1.77	0.42
4:H:13:GLN:HG3	4:H:104:LEU:HA	2.01	0.42
1:A:442:MET:SD	4:D:38:LEU:HD21	2.60	0.42
1:E:183:ILE:HD11	1:E:348:HIS:HB2	2.01	0.42
1:A:94:ALA:O	1:A:98:GLU:HG2	2.19	0.42
1:E:385:SER:O	1:E:386:LEU:C	2.58	0.42
3:G:36:SER:O	3:G:39:THR:OG1	2.32	0.42
2:B:27:ASN:OD1	2:B:27:ASN:N	2.53	0.42
1:E:90:SER:HB3	1:E:93:HIS:NE2	2.35	0.42
1:A:95:TYR:CD2	1:E:60:TYR:HD1	2.38	0.42
4:D:8:VAL:CG1	4:D:9:ASP:H	2.23	0.42
4:D:77:SER:O	4:D:81:THR:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:36:THR:HG23	4:H:36:THR:O	2.20	0.42
4:H:131:LYS:HB2	4:H:132:GLN:NE2	2.35	0.42
1:A:362:GLU:OE2	1:A:379:SER:OG	2.30	0.41
1:E:149:LEU:HD12	1:E:149:LEU:N	2.34	0.41
1:A:110:VAL:HG22	1:A:308:CYS:SG	2.61	0.41
3:G:22:VAL:HG12	3:G:22:VAL:O	2.19	0.41
4:H:23:ASN:HB3	4:H:63:ALA:O	2.19	0.41
4:H:31:SER:HB3	4:H:34:VAL:HG23	2.02	0.41
3:G:5:GLU:HA	3:G:5:GLU:OE1	2.21	0.41
1:A:105:ARG:NH1	1:A:105:ARG:HB2	2.36	0.41
1:A:141:PHE:CZ	1:A:277:ARG:HB3	2.56	0.41
1:A:366:LEU:CD1	1:A:370:LEU:HD11	2.51	0.41
1:E:120:GLU:HG2	1:E:272:ARG:HG2	2.02	0.41
4:H:39:VAL:HG11	4:H:120:ALA:HB2	2.03	0.41
1:A:419:VAL:O	1:A:423:VAL:HG23	2.21	0.41
2:F:53:GLN:HA	2:F:53:GLN:OE1	2.21	0.41
2:F:84:GLU:O	2:F:85:ASN:HB2	2.21	0.41
1:A:318:ASP:O	1:A:322:ILE:HB	2.20	0.40
1:A:401:LEU:N	1:A:401:LEU:HD23	2.35	0.40
4:H:67:THR:HG21	4:H:77:SER:CB	2.51	0.40
1:A:391:VAL:O	1:A:395:ILE:HG23	2.21	0.40
4:D:8:VAL:HG22	4:D:9:ASP:H	1.87	0.40
1:E:70:ASP:O	1:E:73:VAL:N	2.53	0.40
1:E:385:SER:O	1:E:387:GLU:N	2.54	0.40
3:G:36:SER:H	6:G:301:8Q1:P24	2.43	0.40
1:A:155:GLU:OE1	1:A:203:MET:HB3	2.21	0.40
1:E:219:GLY:HA3	1:E:248:LYS:HB2	2.02	0.40
1:E:358:PHE:O	1:E:404:SER:HB3	2.21	0.40
2:F:23:PHE:CD1	2:F:70:VAL:HG22	2.55	0.40
1:A:272:ARG:HE	1:A:272:ARG:HB2	1.59	0.40
1:A:122:ILE:HD13	1:A:291:MET:CB	2.51	0.40
4:H:97:ASN:HB3	4:H:118:GLU:OE2	2.21	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	397/406 (98%)	377 (95%)	16 (4%)	4 (1%)	15	47
1	E	399/406 (98%)	382 (96%)	13 (3%)	4 (1%)	15	47
2	B	79/91 (87%)	77 (98%)	2 (2%)	0	100	100
2	F	81/91 (89%)	80 (99%)	1 (1%)	0	100	100
3	C	69/77 (90%)	62 (90%)	6 (9%)	1 (1%)	11	39
3	G	68/77 (88%)	63 (93%)	5 (7%)	0	100	100
4	D	126/150 (84%)	115 (91%)	6 (5%)	5 (4%)	3	19
4	H	122/150 (81%)	115 (94%)	3 (2%)	4 (3%)	4	23
All	All	1341/1448 (93%)	1271 (95%)	52 (4%)	18 (1%)	12	40

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	273	ARG
1	A	381	CYS
1	E	273	ARG
4	H	18	TYR
4	H	20	ASN
4	H	85	LYS
1	A	275	ARG
1	A	447	ILE
4	D	42	PRO
4	D	45	GLY
3	C	72	ILE
4	D	7	SER
4	D	8	VAL
1	E	274	PRO
1	E	386	LEU
4	H	42	PRO
4	D	32	LYS
1	E	384	ALA

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	292/346 (84%)	289 (99%)	3 (1%)	76	86
1	E	294/346 (85%)	292 (99%)	2 (1%)	84	91
2	B	58/80 (72%)	57 (98%)	1 (2%)	60	79
2	F	60/80 (75%)	59 (98%)	1 (2%)	60	79
3	C	29/66 (44%)	27 (93%)	2 (7%)	15	45
3	G	37/66 (56%)	35 (95%)	2 (5%)	22	54
4	D	61/126 (48%)	61 (100%)	0	100	100
4	H	87/126 (69%)	84 (97%)	3 (3%)	37	66
All	All	918/1236 (74%)	904 (98%)	14 (2%)	65	81

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	GLN
1	A	272	ARG
1	A	277	ARG
2	B	65	VAL
3	C	36	SER
3	C	52	THR
1	E	143	ARG
1	E	172	GLN
2	F	34	ARG
3	G	20	GLU
3	G	36	SER
4	H	13	GLN
4	H	62	ASP
4	H	133	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	GLN
2	B	71	HIS
4	D	23	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)

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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
6	8Q1	G	301	-	27,33,34	1.97	8 (29%)	32,40,43	2.35	10 (31%)
6	8Q1	C	301	3	27,33,34	1.78	5 (18%)	32,40,43	1.71	6 (18%)
5	PLP	E	501	1	15,15,16	1.57	1 (6%)	20,22,23	1.03	2 (10%)
5	PLP	A	501	1	15,15,16	1.60	3 (20%)	20,22,23	1.07	2 (10%)

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
6	8Q1	G	301	-	-	18/38/40/41	-
6	8Q1	C	301	3	-	19/38/40/41	-
5	PLP	E	501	1	-	3/6/6/8	0/1/1/1
5	PLP	A	501	1	-	3/6/6/8	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	301	8Q1	C34-N36	5.37	1.45	1.33
6	C	301	8Q1	C39-N41	5.32	1.45	1.33
6	G	301	8Q1	C39-N41	4.47	1.43	1.33
6	G	301	8Q1	C34-N36	4.30	1.43	1.33
5	E	501	PLP	C5-C4	-4.00	1.36	1.40
5	A	501	PLP	C5-C4	-3.91	1.36	1.40
6	G	301	8Q1	O35-C34	-3.65	1.16	1.23
6	G	301	8Q1	O33-C32	-3.57	1.35	1.42
6	G	301	8Q1	O4-C1	-3.44	1.15	1.21
6	G	301	8Q1	O40-C39	-3.20	1.16	1.23
6	G	301	8Q1	O27-C28	-2.56	1.38	1.44
6	C	301	8Q1	C1-S44	2.39	1.81	1.76
5	A	501	PLP	C3-C2	-2.26	1.38	1.40
6	C	301	8Q1	O35-C34	-2.22	1.19	1.23
6	C	301	8Q1	O40-C39	-2.19	1.18	1.23
5	A	501	PLP	C3-C4	-2.09	1.35	1.40
6	G	301	8Q1	C30-C29	-2.01	1.49	1.53

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	G	301	8Q1	C6-C1-S44	7.65	122.36	113.46
6	C	301	8Q1	C6-C1-S44	5.68	120.06	113.46
6	G	301	8Q1	O4-C1-C6	-4.82	118.30	123.99
6	G	301	8Q1	C31-C29-C32	-4.13	101.66	108.82
6	C	301	8Q1	O4-C1-C6	-3.84	119.46	123.99
6	G	301	8Q1	C37-C38-C39	3.57	118.31	112.36
6	G	301	8Q1	C38-C39-N41	3.53	122.37	116.42
6	G	301	8Q1	C38-C37-N36	-3.35	105.14	111.90
6	C	301	8Q1	C38-C39-N41	2.78	121.11	116.42
6	G	301	8Q1	C43-S44-C1	2.63	110.07	101.87
6	G	301	8Q1	O40-C39-N41	-2.59	118.12	123.01
6	G	301	8Q1	O4-C1-S44	-2.53	119.33	122.61
6	C	301	8Q1	C43-S44-C1	2.51	109.69	101.87
5	A	501	PLP	C6-C5-C4	2.38	120.03	118.16
5	A	501	PLP	C5-C6-N1	-2.35	119.90	123.82
6	C	301	8Q1	C42-N41-C39	-2.25	118.67	122.84
5	E	501	PLP	C6-C5-C4	2.22	119.91	118.16
6	C	301	8Q1	C38-C37-N36	-2.18	107.49	111.90
5	E	501	PLP	C5-C6-N1	-2.14	120.25	123.82
6	G	301	8Q1	C42-N41-C39	-2.02	119.08	122.84

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	PLP	C5A-O4P-P-O2P
5	A	501	PLP	C5A-O4P-P-O3P
5	E	501	PLP	C5A-O4P-P-O1P
5	E	501	PLP	C5A-O4P-P-O2P
5	E	501	PLP	C5A-O4P-P-O3P
6	C	301	8Q1	C1-C6-C7-C8
6	C	301	8Q1	O4-C1-S44-C43
6	C	301	8Q1	C6-C1-S44-C43
6	C	301	8Q1	O27-C28-C29-C30
6	C	301	8Q1	O27-C28-C29-C32
6	C	301	8Q1	C28-C29-C32-C34
6	C	301	8Q1	C28-C29-C32-O33
6	C	301	8Q1	C31-C29-C32-O33
6	C	301	8Q1	N36-C37-C38-C39
6	C	301	8Q1	C42-C43-S44-C1
6	G	301	8Q1	C1-C6-C7-C8
6	G	301	8Q1	O4-C1-S44-C43
6	G	301	8Q1	C6-C1-S44-C43
6	G	301	8Q1	C31-C29-C32-O33
6	G	301	8Q1	N36-C37-C38-C39
6	G	301	8Q1	N41-C42-C43-S44
6	G	301	8Q1	C42-C43-S44-C1
6	C	301	8Q1	O27-C28-C29-C31
6	C	301	8Q1	C7-C8-C9-C10
6	C	301	8Q1	C12-C13-C14-C15
6	G	301	8Q1	C6-C7-C8-C9
6	G	301	8Q1	C7-C8-C9-C10
6	G	301	8Q1	C11-C12-C13-C14
6	G	301	8Q1	C12-C13-C14-C15
6	G	301	8Q1	O33-C32-C34-O35
5	A	501	PLP	C5A-O4P-P-O1P
6	C	301	8Q1	C30-C29-C32-O33
6	G	301	8Q1	C10-C11-C12-C13
6	C	301	8Q1	C30-C29-C32-C34
6	C	301	8Q1	C11-C12-C13-C14
6	G	301	8Q1	C28-C29-C32-O33
6	C	301	8Q1	O33-C32-C34-O35
6	G	301	8Q1	C13-C14-C15-C16
6	C	301	8Q1	C11-C10-C9-C8
6	G	301	8Q1	C29-C32-C34-O35

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Mol	Chain	Res	Type	Atoms
6	G	301	8Q1	C29-C32-C34-N36
6	G	301	8Q1	C11-C10-C9-C8
6	C	301	8Q1	C31-C29-C32-C34

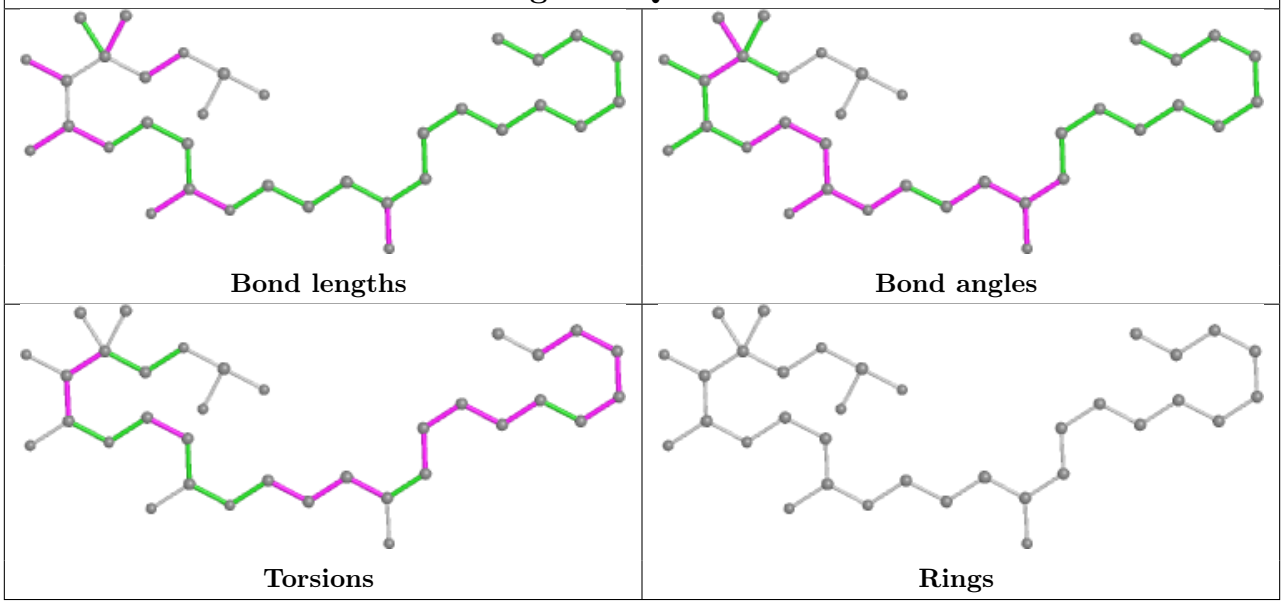
There are no ring outliers.

4 monomers are involved in 10 short contacts:

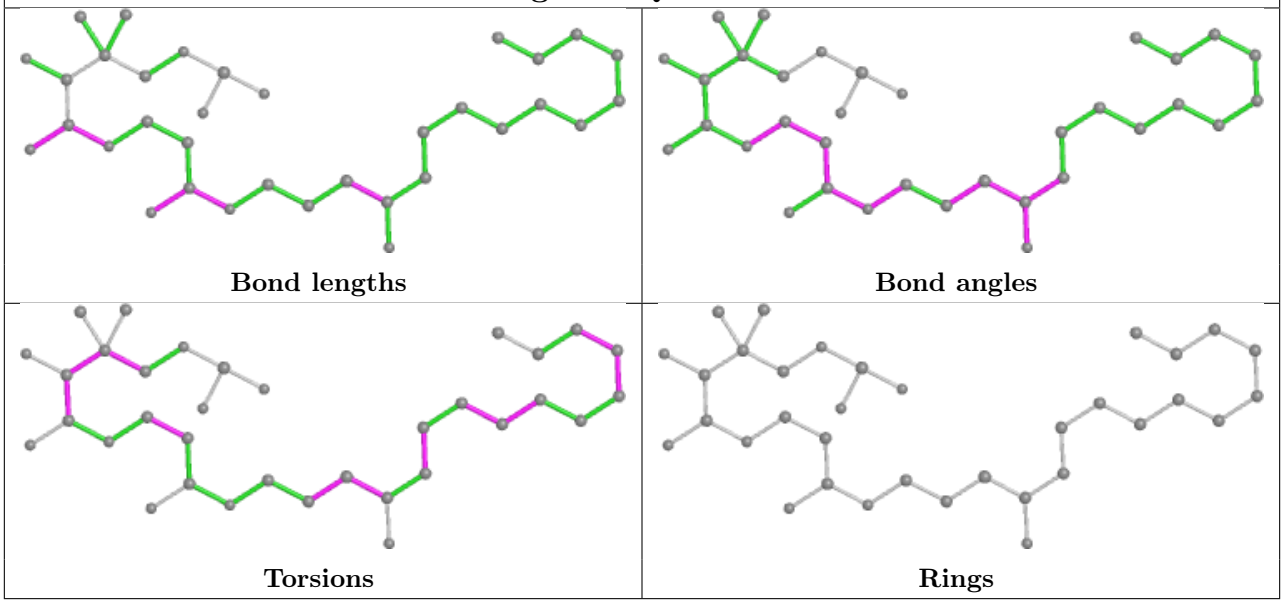
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	301	8Q1	4	0
6	C	301	8Q1	2	0
5	E	501	PLP	2	0
5	A	501	PLP	2	0

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 8Q1 G 301



Ligand 8Q1 C 301



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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	399/406 (98%)	-0.24	0 100 100	47, 69, 109, 154	0
1	E	401/406 (98%)	-0.20	0 100 100	48, 73, 113, 167	0
2	B	81/91 (89%)	-0.23	1 (1%) 79 79	56, 79, 105, 121	0
2	F	83/91 (91%)	-0.35	0 100 100	55, 79, 102, 107	0
3	C	71/77 (92%)	0.35	4 (5%) 24 24	83, 112, 145, 157	0
3	G	70/77 (90%)	-0.04	2 (2%) 51 51	77, 101, 136, 161	0
4	D	128/150 (85%)	0.42	10 (7%) 13 13	90, 121, 154, 179	0
4	H	124/150 (82%)	-0.15	0 100 100	56, 84, 116, 146	0
All	All	1357/1448 (93%)	-0.12	17 (1%) 77 77	47, 78, 134, 179	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	85	ASN	3.2
3	C	22	VAL	3.1
4	D	101	ALA	3.1
4	D	50	LEU	3.0
4	D	38	LEU	3.0
4	D	37	GLY	2.6
4	D	63	ALA	2.4
3	C	52	THR	2.3
4	D	95	ILE	2.3
3	C	26	ALA	2.3
4	D	75	ALA	2.2
4	D	76	SER	2.2
4	D	106	LEU	2.2
4	D	51	GLN	2.1
3	G	54	ILE	2.1
3	G	71	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
3	C	23	THR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

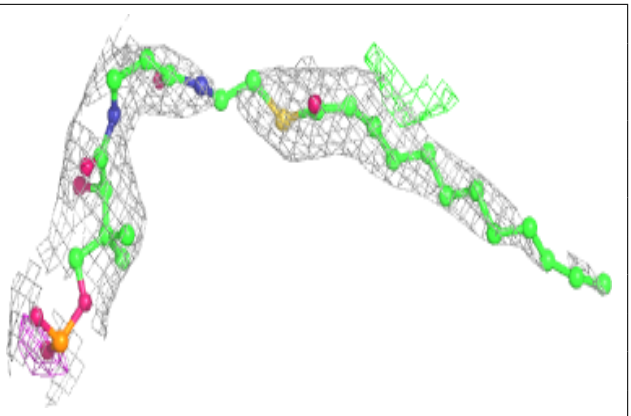
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

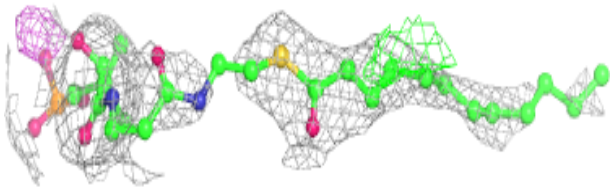
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	8Q1	G	301	34/35	0.91	0.37	74,86,103,110	0
6	8Q1	C	301	34/35	0.92	0.31	71,91,110,115	0
7	ZN	H	201	1/1	0.92	0.14	77,77,77,77	1
7	ZN	D	201	1/1	0.94	0.11	87,87,87,87	1
5	PLP	A	501	15/16	0.94	0.25	62,68,85,101	0
5	PLP	E	501	15/16	0.96	0.20	52,69,81,84	0

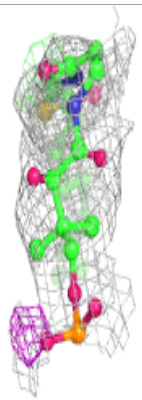
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 8Q1 G 301:

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

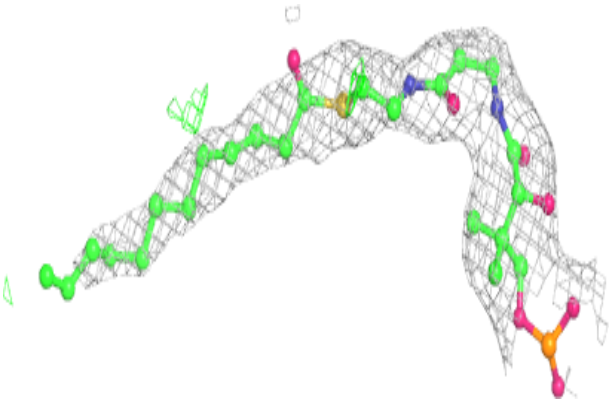


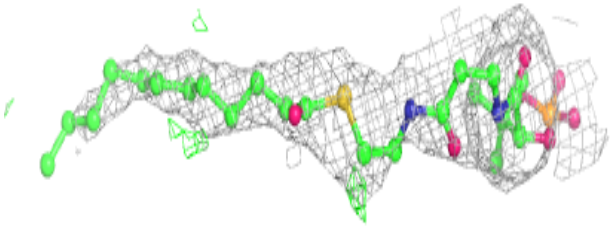


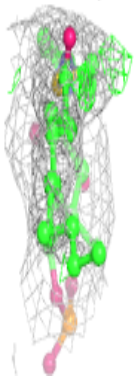


Electron density around 8Q1 C 301:

$2mF_o$-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 (i)

There are no such residues in this entry.