



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:37 PM UTC

PDB ID : 5EXE / pdb_00005exe
Title : Crystal structure of oxalate oxidoreductase from Moorella thermoacetica bound with carboxy-TPP adduct
Authors : Gibson, M.I.; Chen, P.Y.-T.; Drennan, C.L.
Deposited on : 2015-11-23
Resolution : 1.88 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:

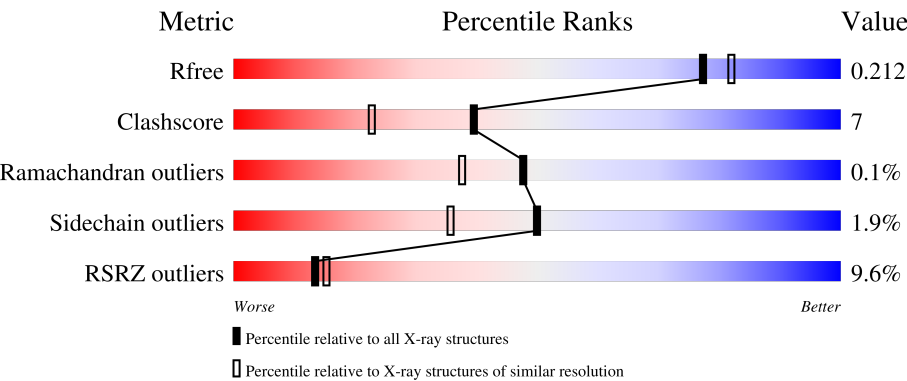
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 1.88 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}	180053	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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 $\leq 5\%$. 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	395	
1	D	395	
2	B	315	
2	E	315	
3	C	314	

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Mol	Chain	Length	Quality of chain
3	F	314	 90%9% •

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 18353 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 Oxalate oxidoreductase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	394	Total	C	N	O	S	0	23	0
			3237	2059	552	611	15			
1	D	394	Total	C	N	O	S	0	24	0
			3245	2064	555	611	15			

- Molecule 2 is a protein called Oxalate oxidoreductase subunit delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	309	Total	C	N	O	S	0	0	0
			2331	1468	394	453	16			
2	E	290	Total	C	N	O	S	0	0	0
			2194	1383	371	425	15			

- Molecule 3 is a protein called Oxalate oxidoreductase subunit beta.

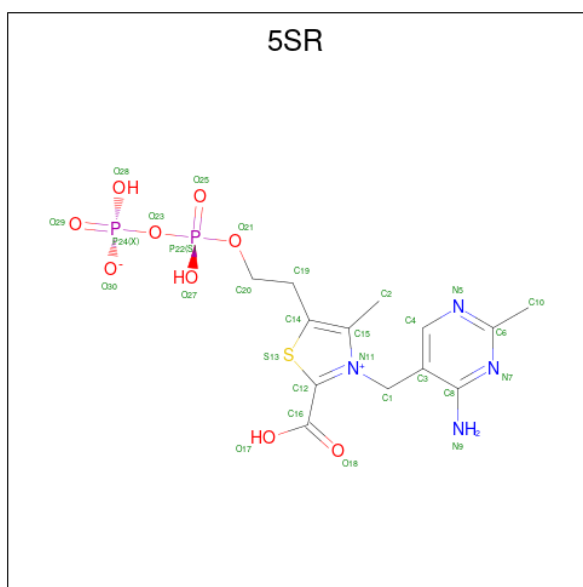
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	314	Total	C	N	O	S	0	0	0
			2406	1542	412	435	17			
3	F	313	Total	C	N	O	S	0	0	0
			2398	1538	410	433	17			

- Molecule 4 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	C	1	Total	Fe	S	0	0
			8	4	4		
4	E	1	Total	Fe	S	0	0
			8	4	4		
4	E	1	Total	Fe	S	0	0
			8	4	4		
4	F	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 5 is [2-[3-[(4-azanyl-2-methyl-pyrimidin-5-yl)methyl]-2-carboxy-4-methyl-1,3-thiazol-3-ium-5-yl]ethoxy-oxidanyl-phosphoryl] hydrogen phosphate (CCD ID: 5SR) (formula: C₁₃H₁₈N₄O₉P₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	P	S	
			29	13	4	9	2	1	0
5	F	1	Total	C	N	O	P	S	
			29	13	4	9	2	1	0

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	2	Total	Mg		
			2	2	0	0
6	F	1	Total	Mg		
			1	1	0	0

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	F	1	Total	Na		
			1	1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	406	Total	O		
			406	406	0	0
8	B	447	Total	O		
			447	447	0	0

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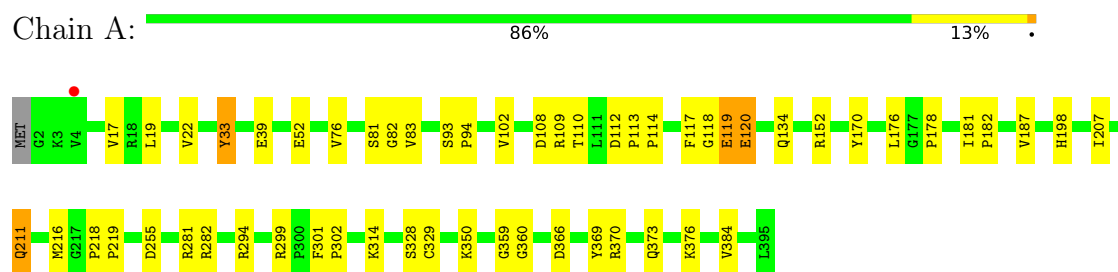
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	380	Total 380	O 380	0	0
8	D	471	Total 471	O 471	0	0
8	E	296	Total 296	O 296	0	0
8	F	432	Total 432	O 432	0	0

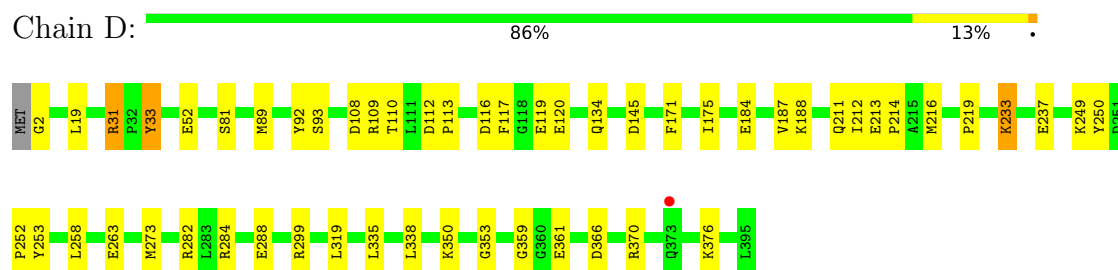
3 Residue-property plots [i](#)

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.

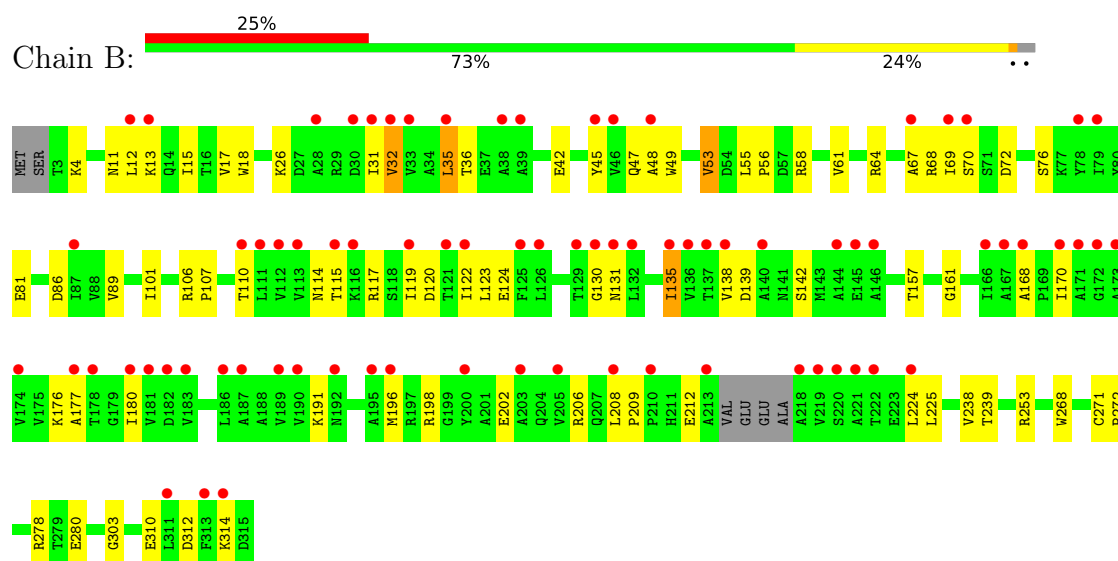
- Molecule 1: Oxalate oxidoreductase subunit alpha



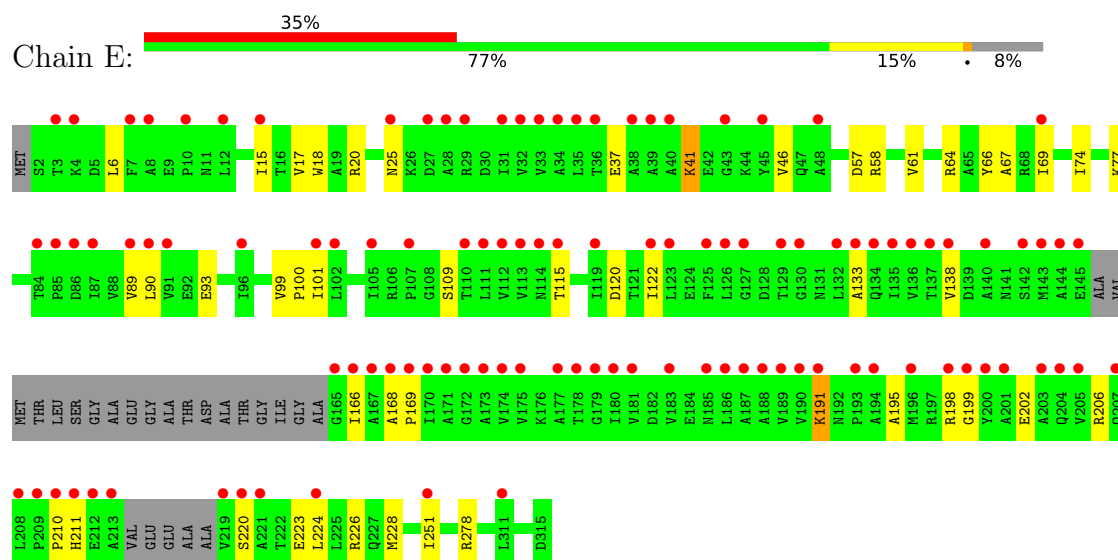
- Molecule 1: Oxalate oxidoreductase subunit alpha



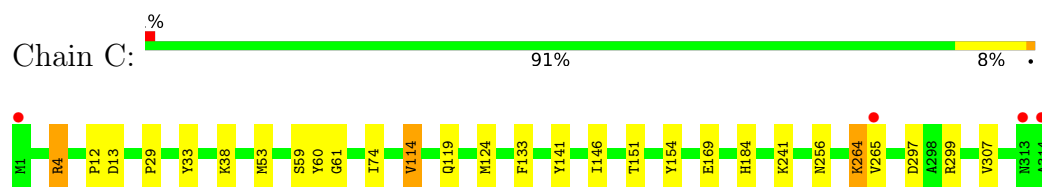
- Molecule 2: Oxalate oxidoreductase subunit delta



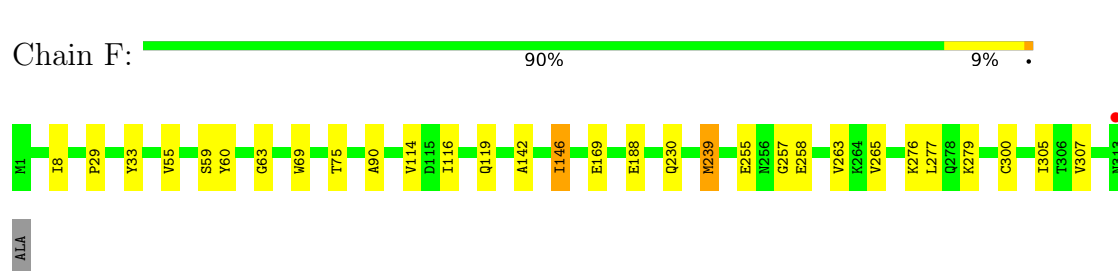
- Molecule 2: Oxalate oxidoreductase subunit delta



- Molecule 3: Oxalate oxidoreductase subunit beta



- Molecule 3: Oxalate oxidoreductase subunit beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	113.65Å 144.13Å 161.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.70 – 1.88 48.70 – 1.88	Depositor EDS
% Data completeness (in resolution range)	92.9 (48.70-1.88) 93.1 (48.70-1.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 1.88Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.181 , 0.213 0.183 , 0.212	Depositor DCC
R_{free} test set	10068 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	22.5	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18353	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 2.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: MG, 5SR, SF4, NA

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	0.38	0/3316	0.69	1/4500 (0.0%)
1	D	0.39	0/3327	0.71	0/4515
2	B	0.39	0/2372	0.77	1/3233 (0.0%)
2	E	0.34	0/2234	0.77	0/3049
3	C	0.40	0/2471	0.72	0/3357
3	F	0.40	0/2463	0.74	0/3346
All	All	0.38	0/16183	0.73	2/22000 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	GLU	N-CA-C	-5.13	101.44	109.38
2	B	209	PRO	O-C-N	5.12	123.67	121.31

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	3237	0	3160	44	0
1	D	3245	0	3173	49	0
2	B	2331	0	2332	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	2194	0	2163	34	0
3	C	2406	0	2405	22	0
3	F	2398	0	2396	20	0
4	B	16	0	0	0	0
4	C	8	0	0	1	0
4	E	16	0	0	0	0
4	F	8	0	0	1	0
5	C	29	0	15	3	0
5	F	29	0	15	2	0
6	C	2	0	0	0	0
6	F	1	0	0	0	0
7	F	1	0	0	0	0
8	A	406	0	0	5	0
8	B	447	0	0	26	1
8	C	380	0	0	9	1
8	D	471	0	0	11	1
8	E	296	0	0	11	0
8	F	432	0	0	7	1
All	All	18353	0	15659	210	2

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 7.

All (210) 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:273:MET:SD	8:D:652:HOH:O	1.96	1.21
1:D:263:GLU:OE1	8:D:401:HOH:O	1.76	1.04
3:F:257:GLY:O	8:F:501:HOH:O	1.81	0.97
3:F:169:GLU:OE1	8:F:502:HOH:O	1.87	0.91
2:B:47:GLN:O	8:B:501:HOH:O	1.90	0.87
1:A:39:GLU:OE1	8:A:401:HOH:O	1.94	0.86
2:B:176:LYS:O	8:B:502:HOH:O	1.92	0.85
2:B:124:GLU:OE1	8:B:503:HOH:O	1.93	0.84
2:B:115:THR:HG21	2:B:122:ILE:HD11	1.58	0.83
2:B:13:LYS:O	8:B:504:HOH:O	1.96	0.83
2:B:31:ILE:O	8:B:505:HOH:O	1.97	0.81
1:A:178:PRO:O	8:A:402:HOH:O	1.97	0.81
2:E:210:PRO:O	8:E:501:HOH:O	1.98	0.80
2:E:109:SER:N	8:E:505:HOH:O	2.13	0.79
1:D:273:MET:HE1	1:D:319:LEU:HD23	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:15:ILE:HB	2:B:67:ALA:HB3	1.63	0.78
3:C:119:GLN:HB2	3:F:119:GLN:HB2	1.65	0.77
2:E:115:THR:HG21	2:E:122:ILE:HD11	1.68	0.76
2:B:48:ALA:HA	8:B:501:HOH:O	1.85	0.76
2:B:310:GLU:OE1	8:B:506:HOH:O	2.03	0.75
1:D:361:GLU:OE2	8:D:402:HOH:O	2.09	0.71
2:B:70:SER:OG	8:B:507:HOH:O	2.09	0.70
1:D:249:LYS:NZ	8:D:404:HOH:O	2.19	0.70
3:C:256:ASN:ND2	8:C:504:HOH:O	2.22	0.69
2:E:93:GLU:OE2	8:E:503:HOH:O	2.10	0.69
2:E:15:ILE:HB	2:E:67:ALA:HB3	1.77	0.66
2:E:223:GLU:OE1	2:E:226:ARG:NH2	2.28	0.66
1:D:282:ARG:NH1	2:E:6:LEU:O	2.29	0.66
1:A:109[B]:ARG:NH2	1:A:112[B]:ASP:OD1	2.22	0.65
2:B:81:GLU:OE1	8:B:508:HOH:O	2.14	0.65
3:C:4:ARG:HG2	8:C:792:HOH:O	1.97	0.65
1:D:31[B]:ARG:NH2	8:D:406:HOH:O	2.25	0.64
2:E:25:ASN:OD1	8:E:506:HOH:O	2.15	0.63
2:B:119:ILE:HG23	2:B:135:ILE:HD12	1.82	0.62
1:D:31[A]:ARG:HG3	8:D:553:HOH:O	2.00	0.62
2:B:117:ARG:NH2	2:B:312:ASP:OD1	2.33	0.61
3:C:299:ARG:NH2	8:C:503:HOH:O	2.22	0.61
2:B:11:ASN:OD1	8:B:509:HOH:O	2.16	0.61
2:B:69:ILE:HG12	2:B:180:ILE:HD11	1.82	0.61
3:C:154:TYR:OH	8:C:501:HOH:O	2.09	0.60
2:B:314:LYS:HG2	8:B:651:HOH:O	2.02	0.60
2:B:198:ARG:NE	2:B:202:GLU:OE1	2.26	0.60
1:D:52:GLU:OE1	8:D:403:HOH:O	2.16	0.59
1:A:110[B]:THR:HG21	1:A:359:GLY:HA2	1.85	0.58
2:B:107:PRO:HA	2:B:131:ASN:HB3	1.85	0.58
1:D:31[A]:ARG:NH1	8:D:415:HOH:O	2.36	0.58
2:E:46:VAL:HG12	2:E:69:ILE:HG12	1.86	0.58
1:D:273:MET:CE	1:D:319:LEU:HD23	2.34	0.58
1:D:109[B]:ARG:NH1	5:F:402:5SR:O18	2.35	0.57
2:B:110:THR:HG21	2:B:177:ALA:HB1	1.85	0.57
2:B:35:LEU:HB2	8:B:505:HOH:O	2.04	0.57
3:C:297:ASP:OD1	8:C:502:HOH:O	2.17	0.57
1:A:19:LEU:HB3	1:A:187:VAL:HG21	1.87	0.57
1:D:110[A]:THR:HG21	1:D:359:GLY:HA2	1.87	0.57
2:E:120:ASP:OD2	2:E:206:ARG:NH1	2.35	0.57
1:D:19:LEU:HB3	1:D:187:VAL:HG21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:ILE:HG13	8:B:504:HOH:O	2.05	0.56
1:A:314:LYS:NZ	8:A:406:HOH:O	2.35	0.56
2:E:90:LEU:HD11	2:E:101:ILE:HD13	1.88	0.56
2:B:130:GLY:O	8:B:510:HOH:O	2.18	0.56
3:C:169:GLU:OE2	8:C:501:HOH:O	2.18	0.56
2:B:114:ASN:HB2	2:B:170:ILE:HD11	1.89	0.55
1:A:118[B]:GLY:HA3	1:A:360:GLY:HA3	1.89	0.55
2:E:20:ARG:HG3	2:E:251:ILE:HD11	1.88	0.55
1:D:134:GLN:HB3	1:D:299:ARG:HB2	1.89	0.54
2:B:224:LEU:HG	1:D:216[B]:MET:HE1	1.89	0.53
1:A:376:LYS:NZ	8:A:409:HOH:O	2.41	0.53
1:A:216[B]:MET:HE1	2:E:224:LEU:HD22	1.91	0.53
2:E:74:ILE:HB	2:E:77:LYS:HE3	1.91	0.53
2:E:278:ARG:NH2	3:F:8:ILE:O	2.41	0.53
1:D:258:LEU:HD13	1:D:284:ARG:HG3	1.91	0.52
2:B:53:VAL:HG11	1:D:214[B]:PRO:HG3	1.90	0.52
1:A:110[B]:THR:HB	1:A:114[B]:PRO:HD2	1.92	0.52
2:B:45:TYR:N	2:B:70:SER:O	2.32	0.52
1:D:366:ASP:O	1:D:370:ARG:HG3	2.10	0.52
2:E:198:ARG:NE	8:E:502:HOH:O	2.08	0.52
2:B:12:LEU:O	2:B:106:ARG:NH2	2.44	0.51
1:A:366:ASP:O	1:A:370:ARG:HG3	2.10	0.51
1:D:31[B]:ARG:NE	1:D:117[B]:PHE:HB3	2.26	0.51
3:C:124:MET:HE1	3:C:133:PHE:HB2	1.93	0.50
2:B:42:GLU:OE1	8:B:511:HOH:O	2.18	0.50
2:E:191:LYS:NZ	8:E:519:HOH:O	2.44	0.50
1:D:213[B]:GLU:HG2	1:D:216[B]:MET:HG2	1.92	0.50
1:A:109[B]:ARG:NH1	1:A:110[B]:THR:O	2.45	0.50
2:B:123:LEU:O	8:B:513:HOH:O	2.20	0.50
2:E:211:HIS:HA	8:E:501:HOH:O	2.12	0.49
2:B:36:THR:HG21	8:B:501:HOH:O	2.12	0.49
1:A:170:TYR:HH	2:B:49:TRP:CD1	2.30	0.49
2:B:278:ARG:HD3	3:C:13:ASP:OD1	2.11	0.49
2:B:48:ALA:N	8:B:516:HOH:O	2.25	0.49
1:A:109[A]:ARG:HA	1:A:119[A]:GLU:HA	1.95	0.49
1:D:188:LYS:NZ	8:D:419:HOH:O	2.41	0.49
3:C:264:LYS:HG3	8:C:691:HOH:O	2.13	0.48
1:D:233:LYS:NZ	1:D:237:GLU:OE2	2.45	0.48
1:D:33:TYR:HB3	1:D:81:SER:OG	2.13	0.48
3:C:29:PRO:HG2	4:C:401:SF4:S4	2.53	0.48
1:A:52:GLU:HG2	3:F:90:ALA:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:196:MET:HE3	2:B:196:MET:HB3	1.77	0.48
3:F:258:GLU:HA	8:F:501:HOH:O	2.14	0.48
3:F:276:LYS:HD3	8:F:722:HOH:O	2.13	0.48
1:A:82:GLY:HA3	1:A:109[B]:ARG:HH11	1.78	0.47
3:C:61:GLY:N	1:D:211[B]:GLN:O	2.34	0.47
1:A:108[A]:ASP:HB3	1:A:120:GLU:O	2.14	0.47
2:B:18:TRP:CH2	2:B:64:ARG:HD3	2.50	0.47
2:B:120:ASP:O	2:B:124:GLU:HG2	2.15	0.47
1:A:211[B]:GLN:HE21	1:A:211[B]:GLN:HB2	1.58	0.47
2:E:41:LYS:HB2	2:E:41:LYS:HE2	1.64	0.47
1:A:117[B]:PHE:HB2	8:D:566:HOH:O	2.15	0.47
2:E:66:TYR:OH	8:E:504:HOH:O	2.10	0.47
2:B:117:ARG:HB2	8:B:518:HOH:O	2.14	0.46
2:E:191:LYS:O	2:E:191:LYS:HD3	2.15	0.46
1:D:109[A]:ARG:NE	1:D:116[A]:ASP:HA	2.30	0.46
3:C:241:LYS:NZ	8:C:510:HOH:O	2.46	0.46
3:F:142:ALA:HA	3:F:146:ILE:HD13	1.97	0.46
3:F:239:MET:HE1	3:F:277:LEU:HB2	1.98	0.46
2:B:206:ARG:NH1	8:B:531:HOH:O	2.46	0.46
1:A:176:LEU:HD12	2:B:48:ALA:HB3	1.98	0.46
3:C:241:LYS:NZ	8:C:507:HOH:O	2.37	0.46
1:A:216[A]:MET:HB3	2:E:228:MET:CE	2.45	0.46
1:A:76:VAL:HG21	1:A:102:VAL:HG22	1.98	0.46
1:A:216[A]:MET:C	1:A:219[A]:PRO:HD2	2.41	0.46
3:C:141:TYR:HD1	5:C:402:5SR:H13	1.81	0.46
1:A:207:ILE:HD13	3:F:63:GLY:HA3	1.96	0.46
2:B:191:LYS:NZ	8:B:519:HOH:O	2.30	0.46
3:F:29:PRO:HG2	4:F:401:SF4:S4	2.57	0.45
2:E:41:LYS:HD3	8:E:517:HOH:O	2.16	0.45
2:B:26:LYS:NZ	2:B:161:GLY:O	2.49	0.45
2:B:68:ARG:NH1	2:B:76:SER:OG	2.50	0.45
2:B:238:VAL:HG12	2:B:239:THR:HG23	1.97	0.45
3:C:59:SER:HA	3:C:60:TYR:HA	1.73	0.45
2:E:18:TRP:CZ2	2:E:64:ARG:HD3	2.51	0.45
3:F:265:VAL:O	3:F:307:VAL:HG11	2.17	0.45
3:F:188:GLU:OE2	8:F:503:HOH:O	2.21	0.45
5:C:402:5SR:C16	5:C:402:5SR:H10	2.29	0.45
2:E:133:ALA:N	8:E:505:HOH:O	2.50	0.45
3:F:255:GLU:OE2	8:F:504:HOH:O	2.21	0.45
1:A:113[A]:PRO:HD3	1:D:93:SER:O	2.17	0.44
1:A:301:PHE:HA	1:A:302:PRO:HD3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:280:GLU:HG3	8:B:539:HOH:O	2.16	0.44
1:A:112[A]:ASP:O	1:D:93:SER:OG	2.29	0.44
1:D:89:MET:HA	1:D:92:TYR:CE2	2.52	0.44
1:D:184:GLU:OE1	1:D:184:GLU:N	2.46	0.44
1:A:33:TYR:HB3	1:A:81:SER:OG	2.18	0.44
2:B:55:LEU:HA	2:B:56:PRO:C	2.43	0.44
2:E:169:PRO:HG3	2:E:195:ALA:HB1	2.00	0.44
1:A:83:VAL:HG13	1:A:109[B]:ARG:HH12	1.82	0.44
1:A:94:PRO:HA	1:D:113[B]:PRO:HG3	2.00	0.44
1:D:81:SER:HB3	1:D:109[A]:ARG:HB2	2.00	0.44
1:D:108[B]:ASP:HB3	1:D:120:GLU:O	2.18	0.44
2:E:168:ALA:HB3	2:E:169:PRO:HD3	1.98	0.44
1:A:134:GLN:HB3	1:A:299:ARG:HB2	1.98	0.44
2:B:70:SER:OG	2:B:72:ASP:O	2.32	0.44
1:D:184:GLU:O	1:D:188:LYS:HG2	2.17	0.44
2:E:58:ARG:O	2:E:61:VAL:HG12	2.18	0.44
1:A:281:ARG:HH22	1:A:282:ARG:HE	1.66	0.44
2:B:225:LEU:HA	1:D:219[A]:PRO:HB3	1.99	0.43
2:B:58:ARG:O	2:B:61:VAL:HG12	2.18	0.43
2:B:139:ASP:OD2	2:B:142:SER:OG	2.31	0.43
2:B:253:ARG:NH2	2:B:310:GLU:OE1	2.46	0.43
3:C:29:PRO:HB2	3:C:53:MET:HE3	2.00	0.43
1:A:17:VAL:HG13	1:A:22:VAL:HG21	2.01	0.43
2:B:303:GLY:HA2	8:B:540:HOH:O	2.19	0.43
1:D:145:ASP:OD2	1:D:250:TYR:OH	2.31	0.43
3:F:59:SER:HA	3:F:60:TYR:HA	1.69	0.43
2:E:166:ILE:C	2:E:169:PRO:HD2	2.43	0.43
1:D:335:LEU:HD22	1:D:353:GLY:HA3	2.01	0.43
1:D:89:MET:HA	1:D:92:TYR:CD2	2.54	0.42
1:A:114[A]:PRO:HG2	1:D:212[A]:ILE:HG23	2.01	0.42
1:A:281:ARG:HH11	1:A:281:ARG:HB3	1.85	0.42
2:B:32:VAL:HA	8:B:505:HOH:O	2.20	0.42
8:A:401:HOH:O	2:B:157:THR:N	2.36	0.42
2:B:168:ALA:HB1	2:B:196:MET:HB2	2.01	0.42
3:C:114:VAL:HG21	3:C:151:THR:HG23	2.01	0.42
2:E:17:VAL:HG22	2:E:89:VAL:HB	2.02	0.42
2:E:37:GLU:O	8:E:507:HOH:O	2.21	0.42
1:A:350:LYS:HE3	1:A:384:VAL:HG23	2.02	0.42
2:B:17:VAL:HG22	2:B:89:VAL:HB	2.02	0.42
3:F:75:THR:HG22	3:F:116:ILE:HG12	2.02	0.42
1:A:211[B]:GLN:NE2	3:F:55:VAL:HG22	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:268:TRP:CE2	2:B:278:ARG:HD2	2.54	0.41
1:A:181:ILE:HA	1:A:182:PRO:HD3	1.92	0.41
2:E:199:GLY:HA2	2:E:202:GLU:HB2	2.02	0.41
3:F:230:GLN:HB2	3:F:279:LYS:HB2	2.01	0.41
1:D:2:GLY:N	8:D:435:HOH:O	2.53	0.41
1:A:93:SER:OG	1:D:112[B]:ASP:O	2.32	0.41
2:E:57:ASP:OD2	2:E:57:ASP:N	2.49	0.41
2:B:13:LYS:HA	2:B:86:ASP:OD1	2.20	0.41
1:A:218[B]:PRO:HG2	1:D:361:GLU:HG3	2.03	0.41
1:A:369:TYR:O	1:A:373:GLN:HG2	2.21	0.41
2:E:99:VAL:HA	2:E:100:PRO:HD3	1.88	0.41
3:C:74:ILE:HD12	5:C:402:5SR:H16	2.03	0.41
1:A:207:ILE:HG23	3:F:69:TRP:CE3	2.56	0.41
1:A:255:ASP:HB3	1:A:294:ARG:HB3	2.02	0.41
2:B:26:LYS:HB3	8:B:618:HOH:O	2.21	0.41
3:C:12:PRO:O	3:C:38:LYS:NZ	2.52	0.41
3:C:265:VAL:O	3:C:307:VAL:HG11	2.21	0.41
1:D:213[B]:GLU:HB2	1:D:214[B]:PRO:HD2	2.02	0.41
1:D:252:PRO:HG2	1:D:253:TYR:CE2	2.55	0.41
1:D:288:GLU:OE1	1:D:376:LYS:NZ	2.50	0.41
1:D:350:LYS:HA	1:D:350:LYS:HD3	1.85	0.41
2:B:239:THR:HG22	8:B:692:HOH:O	2.22	0.40
3:C:184:HIS:HD2	8:F:509:HOH:O	2.04	0.40
2:B:18:TRP:CZ2	2:B:64:ARG:HD3	2.56	0.40
1:D:171:PHE:HA	1:D:175:ILE:HD12	2.04	0.40
1:D:108[A]:ASP:HB3	1:D:120:GLU:O	2.21	0.40
1:D:212[A]:ILE:HB	1:D:216[A]:MET:HB2	2.03	0.40
3:F:300:CYS:HB3	3:F:305:ILE:HB	2.02	0.40
1:A:328:SER:O	1:A:329:CYS:HB2	2.22	0.40
2:B:271:CYS:HA	2:B:272:PRO:HD3	1.95	0.40
5:F:402:5SR:O18	5:F:402:5SR:H2	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:860:HOH:O	8:D:838:HOH:O[2_455]	1.95	0.25
8:B:529:HOH:O	8:F:773:HOH:O[3_555]	2.11	0.09

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	415/395 (105%)	405 (98%)	10 (2%)	0	100	100
1	D	416/395 (105%)	402 (97%)	14 (3%)	0	100	100
2	B	305/315 (97%)	297 (97%)	8 (3%)	0	100	100
2	E	284/315 (90%)	274 (96%)	10 (4%)	0	100	100
3	C	312/314 (99%)	301 (96%)	10 (3%)	1 (0%)	36	26
3	F	311/314 (99%)	298 (96%)	12 (4%)	1 (0%)	36	26
All	All	2043/2048 (100%)	1977 (97%)	64 (3%)	2 (0%)	48	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	146	ILE
3	F	146	ILE

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	339/322 (105%)	332 (98%)	7 (2%)	47	32
1	D	340/322 (106%)	333 (98%)	7 (2%)	47	32
2	B	251/256 (98%)	242 (96%)	9 (4%)	31	14
2	E	236/256 (92%)	232 (98%)	4 (2%)	53	40
3	C	250/250 (100%)	246 (98%)	4 (2%)	55	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	249/250 (100%)	245 (98%)	4 (2%)	55	43
All	All	1665/1656 (100%)	1630 (98%)	35 (2%)	50	32

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	TYR
1	A	119[A]	GLU
1	A	119[B]	GLU
1	A	152	ARG
1	A	198	HIS
1	A	211[A]	GLN
1	A	211[B]	GLN
2	B	4	LYS
2	B	32	VAL
2	B	35	LEU
2	B	53	VAL
2	B	101	ILE
2	B	135	ILE
2	B	138	VAL
2	B	208	LEU
2	B	212	GLU
3	C	4	ARG
3	C	33	TYR
3	C	114	VAL
3	C	264	LYS
1	D	31[A]	ARG
1	D	31[B]	ARG
1	D	33	TYR
1	D	119[A]	GLU
1	D	119[B]	GLU
1	D	233	LYS
1	D	338	LEU
2	E	41	LYS
2	E	138	VAL
2	E	191	LYS
2	E	220	SER
3	F	33	TYR
3	F	114	VAL
3	F	239	MET
3	F	263	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	HIS
3	C	73	GLN
3	C	184	HIS
1	D	373	GLN
3	F	73	GLN
3	F	184	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	$\# Z > 2$
4	SF4	F	401	3	0,12,12	-	-	-		
5	5SR	F	402	6	29,30,30	1.90	6 (20%)	36,45,45	1.45	7 (19%)
4	SF4	E	401	2	0,12,12	-	-	-		
4	SF4	B	402	2	0,12,12	-	-	-		
4	SF4	E	402	2	0,12,12	-	-	-		
4	SF4	C	401	3	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	5SR	C	402	6	29,30,30	1.97	7 (24%)	36,45,45	1.46	6 (16%)
4	SF4	B	401	2	0,12,12	-	-	-		

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
4	SF4	F	401	3	-	-	0/6/5/5
5	5SR	F	402	6	-	1/19/21/21	0/2/2/2
4	SF4	E	401	2	-	-	0/6/5/5
4	SF4	B	402	2	-	-	0/6/5/5
4	SF4	E	402	2	-	-	0/6/5/5
4	SF4	C	401	3	-	-	0/6/5/5
5	5SR	C	402	6	-	2/19/21/21	0/2/2/2
4	SF4	B	401	2	-	-	0/6/5/5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	402	5SR	C8-N9	5.66	1.48	1.34
5	C	402	5SR	C8-N9	5.65	1.48	1.34
5	C	402	5SR	C14-S13	5.45	1.85	1.74
5	F	402	5SR	C14-S13	4.72	1.83	1.74
5	C	402	5SR	C12-S13	3.67	1.84	1.71
5	F	402	5SR	C12-S13	3.62	1.84	1.71
5	C	402	5SR	C12-N11	2.97	1.42	1.34
5	C	402	5SR	O18-C16	2.92	1.29	1.22
5	F	402	5SR	C12-N11	2.92	1.42	1.34
5	C	402	5SR	C3-C8	-2.90	1.38	1.42
5	F	402	5SR	C3-C8	-2.84	1.38	1.42
5	F	402	5SR	O18-C16	2.80	1.29	1.22
5	C	402	5SR	P22-O23	2.52	1.62	1.59

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	402	5SR	N5-C6-N7	-3.23	120.16	125.53
5	F	402	5SR	N5-C6-N7	-3.14	120.31	125.53
5	C	402	5SR	C4-C3-C8	2.97	119.20	115.55
5	F	402	5SR	C4-N5-C6	2.93	120.88	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	402	5SR	C4-C3-C8	2.86	119.07	115.55
5	C	402	5SR	C4-N5-C6	2.85	120.75	116.07
5	C	402	5SR	C3-C4-N5	-2.62	119.57	123.83
5	F	402	5SR	N9-C8-N7	2.61	120.55	117.03
5	F	402	5SR	C3-C4-N5	-2.54	119.69	123.83
5	C	402	5SR	C10-C6-N5	2.41	119.76	117.20
5	C	402	5SR	N9-C8-N7	2.39	120.25	117.03
5	F	402	5SR	C10-C6-N7	2.27	120.52	117.13
5	F	402	5SR	O30-P24-O28	2.16	115.89	107.80

There are no chirality outliers.

All (3) torsion outliers are listed below:

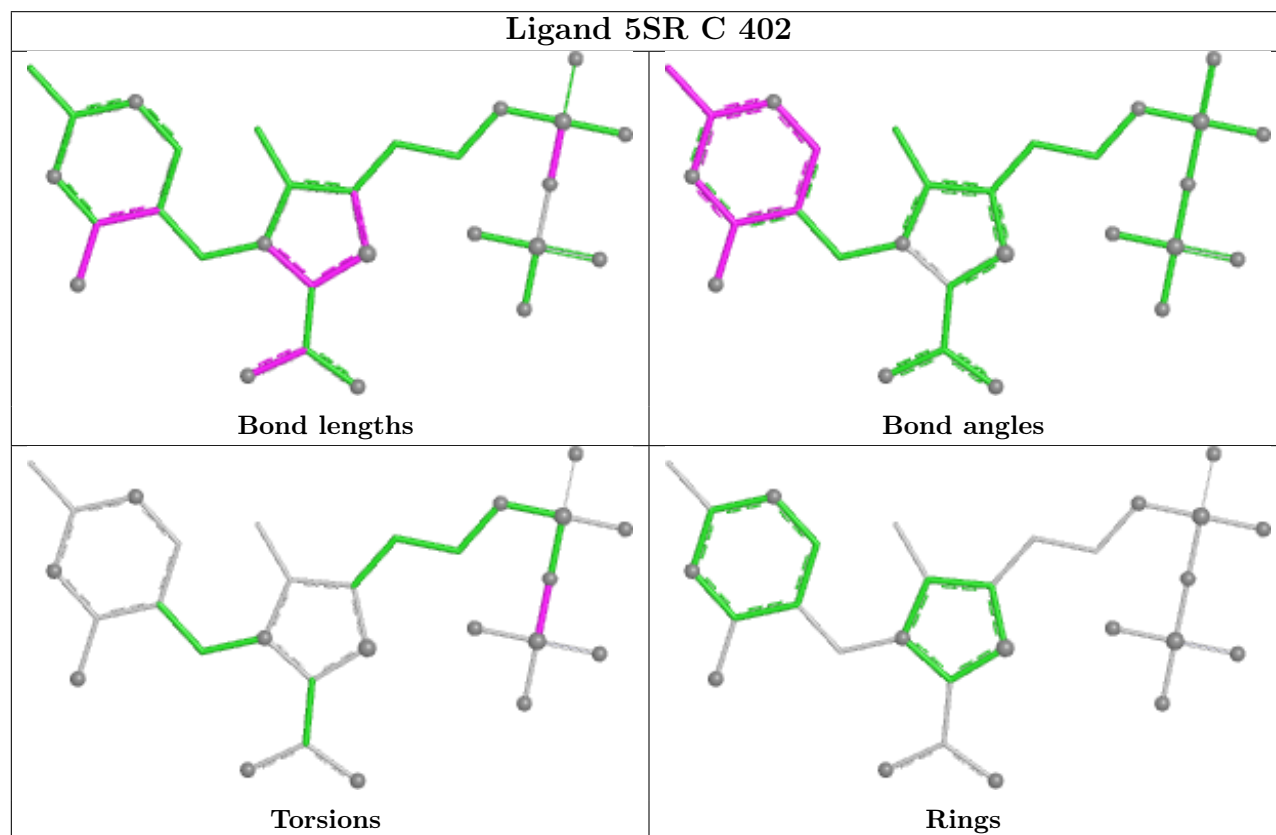
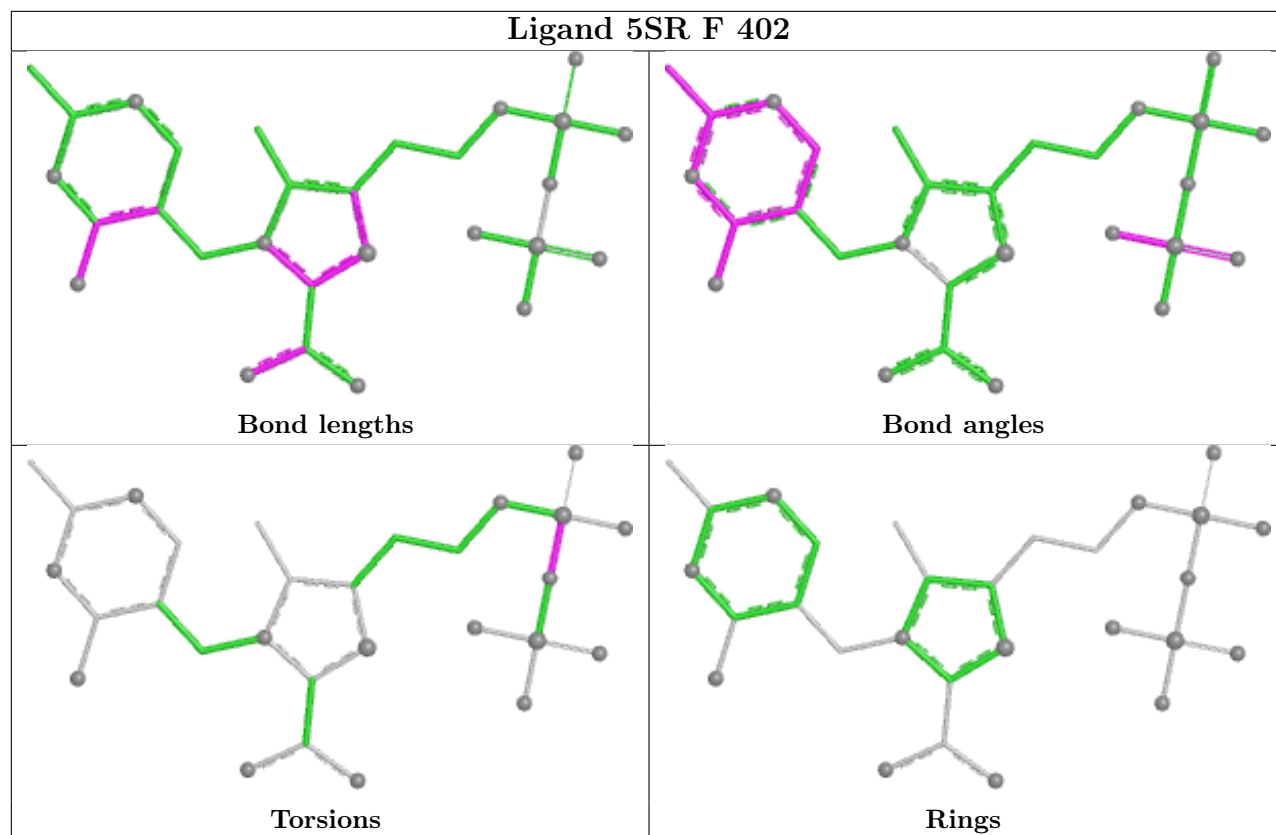
Mol	Chain	Res	Type	Atoms
5	C	402	5SR	P22-O23-P24-O30
5	F	402	5SR	P24-O23-P22-O21
5	C	402	5SR	P22-O23-P24-O28

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	401	SF4	1	0
5	F	402	5SR	2	0
4	C	401	SF4	1	0
5	C	402	5SR	3	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 than 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.



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, 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	394/395 (99%)	-0.33	1 (0%) 90 93	9, 22, 38, 50	23 (5%)
1	D	394/395 (99%)	-0.27	1 (0%) 90 93	9, 22, 39, 53	24 (6%)
2	B	309/315 (98%)	1.16	78 (25%) 1 1	15, 38, 60, 93	0
2	E	290/315 (92%)	1.56	109 (37%) 1 0	19, 48, 74, 105	0
3	C	314/314 (100%)	-0.38	4 (1%) 75 80	14, 20, 40, 72	0
3	F	313/314 (99%)	-0.35	1 (0%) 90 93	15, 21, 37, 49	0
All	All	2014/2048 (98%)	0.17	194 (9%) 13 15	9, 24, 60, 105	47 (2%)

All (194) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	186	LEU	5.8
2	E	201	ALA	5.7
2	E	210	PRO	4.9
2	B	218	ALA	4.8
3	C	314	ALA	4.8
2	B	171	ALA	4.8
2	E	171	ALA	4.7
2	B	181	VAL	4.7
2	E	110	THR	4.6
2	B	213	ALA	4.5
2	E	175	VAL	4.4
2	E	111	LEU	4.4
2	E	180	ILE	4.4
2	E	166	ILE	4.4
2	E	181	VAL	4.3
2	E	135	ILE	4.3
2	B	170	ILE	4.3
2	E	38	ALA	4.3
2	E	3	THR	4.3

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Mol	Chain	Res	Type	RSRZ
2	E	138	VAL	4.3
2	B	219	VAL	4.2
2	E	205	VAL	4.2
2	B	136	VAL	4.1
2	B	69	ILE	4.1
2	E	219	VAL	4.1
2	E	174	VAL	4.0
2	B	221	ALA	4.0
2	E	126	LEU	4.0
2	E	213	ALA	4.0
2	B	111	LEU	4.0
2	B	32	VAL	4.0
2	B	135	ILE	4.0
2	B	205	VAL	4.0
2	E	189	VAL	3.9
2	B	140	ALA	3.9
2	E	112	VAL	3.8
2	B	195	ALA	3.8
2	E	39	ALA	3.7
2	E	35	LEU	3.7
2	E	34	ALA	3.7
2	E	105	ILE	3.7
2	B	113	VAL	3.7
2	B	172	GLY	3.7
2	E	221	ALA	3.6
2	B	177	ALA	3.6
2	E	144	ALA	3.6
2	B	166	ILE	3.6
2	E	130	GLY	3.6
2	E	199	GLY	3.6
2	B	112	VAL	3.6
2	B	190	VAL	3.6
2	B	48	ALA	3.5
2	B	222	THR	3.5
2	E	122	ILE	3.5
2	E	32	VAL	3.5
2	E	43	GLY	3.5
2	E	169	PRO	3.5
2	B	174	VAL	3.5
2	B	183	VAL	3.5
2	E	177	ALA	3.5
2	E	129	THR	3.5

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Mol	Chain	Res	Type	RSRZ
2	E	69	ILE	3.5
2	E	188	ALA	3.4
2	B	35	LEU	3.4
2	B	132	LEU	3.4
2	E	136	VAL	3.4
2	E	90	LEU	3.4
2	E	15	ILE	3.4
2	E	165	GLY	3.4
2	E	12	LEU	3.3
2	E	209	PRO	3.3
2	E	211	HIS	3.3
2	B	31	ILE	3.3
2	B	180	ILE	3.3
2	E	183	VAL	3.3
2	E	132	LEU	3.3
2	B	125	PHE	3.3
2	E	89	VAL	3.2
2	E	178	THR	3.2
2	E	91	VAL	3.2
2	E	190	VAL	3.2
2	E	102	LEU	3.1
2	E	40	ALA	3.1
2	E	29	ARG	3.1
2	B	144	ALA	3.1
2	E	127	GLY	3.1
1	A	4	VAL	3.0
2	B	187	ALA	3.0
2	E	119	ILE	3.0
2	E	200	TYR	3.0
2	B	138	VAL	3.0
2	E	10	PRO	3.0
2	E	31	ILE	3.0
2	E	220	SER	2.9
2	E	27	ASP	2.9
2	B	38	ALA	2.9
2	E	168	ALA	2.9
2	E	87	ILE	2.9
2	E	208	LEU	2.9
2	E	224	LEU	2.9
2	E	170	ILE	2.9
2	B	46	VAL	2.9
2	B	178	THR	2.9

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Mol	Chain	Res	Type	RSRZ
3	C	313	ASN	2.9
2	B	168	ALA	2.9
2	E	140	ALA	2.9
2	E	167	ALA	2.9
2	B	79	ILE	2.9
2	B	208	LEU	2.9
3	C	265	VAL	2.8
2	B	200	TYR	2.8
2	B	116	LYS	2.8
2	B	122	ILE	2.8
2	E	212	GLU	2.8
2	E	28	ALA	2.8
2	B	119	ILE	2.8
2	E	193	PRO	2.8
2	E	113	VAL	2.8
2	E	196	MET	2.8
2	B	30	ASP	2.8
2	B	131	ASN	2.7
2	E	203	ALA	2.7
2	E	125	PHE	2.7
2	E	145	GLU	2.7
2	E	187	ALA	2.7
2	B	130	GLY	2.7
2	B	182	ASP	2.6
2	E	123	LEU	2.6
2	B	196	MET	2.6
2	E	86	ASP	2.6
2	B	33	VAL	2.6
2	B	173	ALA	2.6
2	E	101	ILE	2.5
2	B	28	ALA	2.5
2	B	39	ALA	2.5
2	B	121	THR	2.5
3	C	1	MET	2.5
3	F	313	ASN	2.5
2	B	146	ALA	2.5
2	B	167	ALA	2.5
2	E	173	ALA	2.5
2	E	134	GLN	2.5
2	E	137	THR	2.5
2	E	107	PRO	2.5
2	E	45	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	224	LEU	2.4
2	B	110	THR	2.4
2	B	129	THR	2.4
2	B	203	ALA	2.4
2	E	8	ALA	2.4
2	E	194	ALA	2.4
2	E	25	ASN	2.4
2	B	220	SER	2.4
2	E	7	PHE	2.4
2	E	4	LYS	2.4
2	E	251	ILE	2.4
2	B	311	LEU	2.4
2	E	133	ALA	2.4
2	E	33	VAL	2.4
2	E	172	GLY	2.4
2	B	313	PHE	2.3
2	E	36	THR	2.3
2	B	87	ILE	2.3
2	E	85	PRO	2.3
2	E	143	MET	2.3
2	B	12	LEU	2.3
2	B	67	ALA	2.3
2	B	189	VAL	2.3
2	E	84	THR	2.3
2	B	45	TYR	2.3
2	E	96	ILE	2.3
2	B	145	GLU	2.3
2	B	137	THR	2.3
2	B	314	LYS	2.3
2	B	192	ASN	2.2
2	E	198	ARG	2.2
2	B	70	SER	2.2
2	E	142	SER	2.2
2	B	210	PRO	2.2
2	E	204	GLN	2.2
2	B	13	LYS	2.2
2	E	191	LYS	2.2
2	E	114	ASN	2.1
2	B	78	TYR	2.1
2	E	311	LEU	2.1
1	D	373	GLN	2.1
2	B	126	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	115	THR	2.1
2	E	179	GLY	2.1
2	B	186	LEU	2.1
2	E	185	ASN	2.0
2	E	48	ALA	2.0
2	B	115	THR	2.0
2	E	207	GLN	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

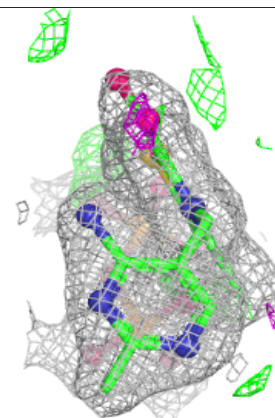
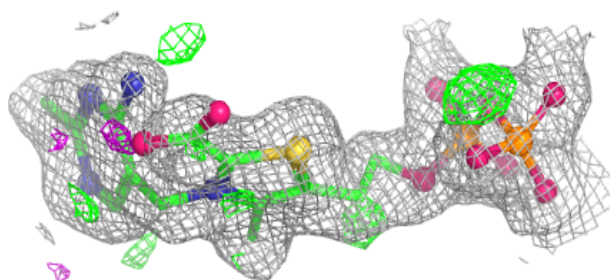
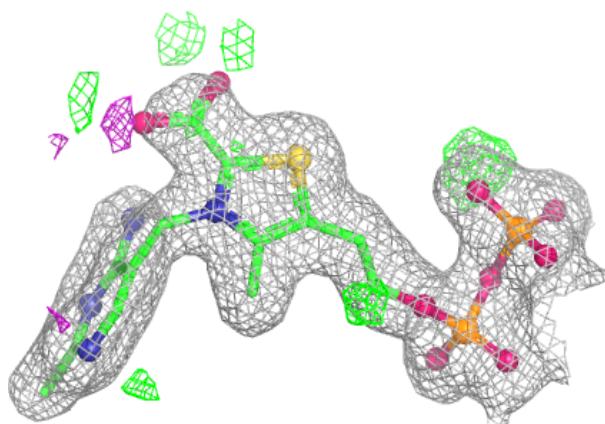
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	MG	C	404	1/1	0.96	0.06	33,33,33,33	0
7	NA	F	404	1/1	0.96	0.06	28,28,28,28	0
5	5SR	F	402	29/29	0.98	0.06	14,18,23,32	3
4	SF4	E	401	8/8	0.98	0.03	19,22,23,23	0
5	5SR	C	402	29/29	0.98	0.05	12,18,24,28	3
4	SF4	F	401	8/8	0.99	0.03	18,19,22,23	0
4	SF4	B	402	8/8	0.99	0.02	17,18,19,22	0
4	SF4	C	401	8/8	0.99	0.03	15,16,17,18	0
6	MG	C	403	1/1	0.99	0.04	13,13,13,13	0
4	SF4	B	401	8/8	0.99	0.03	17,18,19,20	0
6	MG	F	403	1/1	0.99	0.05	15,15,15,15	0
4	SF4	E	402	8/8	0.99	0.03	22,22,23,27	0

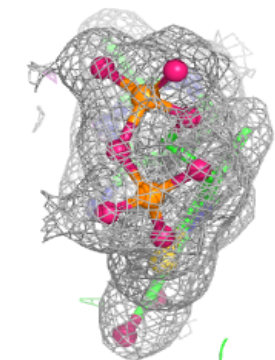
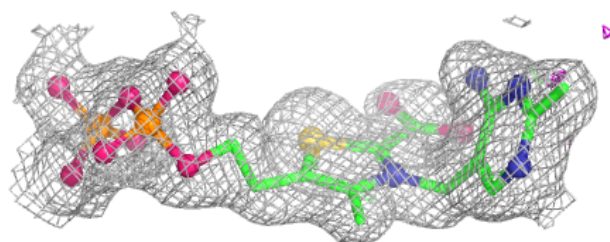
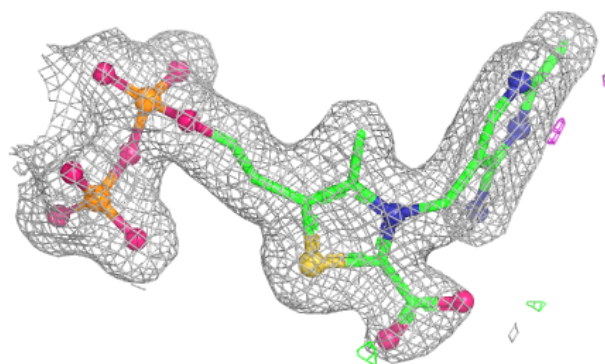
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 5SR F 402:

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

**Electron density around 5SR C 402:**

$2mF_o-DF_c$ (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.