



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 02:30 PM UTC

PDB ID : 5X3R / pdb_00005x3r
Title : Crystal structure of the SmcR complexed with QStatin
Authors : Jang, S.Y.; Hwang, J.; Kim, M.H.
Deposited on : 2017-02-07
Resolution : 2.10 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

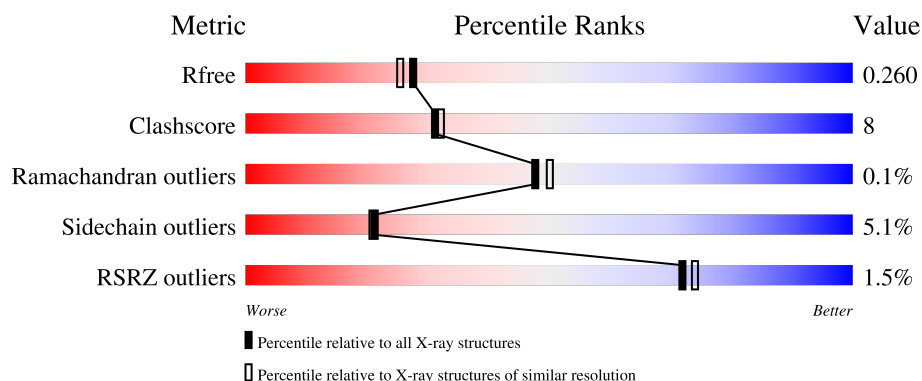
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	205	
1	B	205	
1	C	205	
1	D	205	

2 Entry composition [i](#)

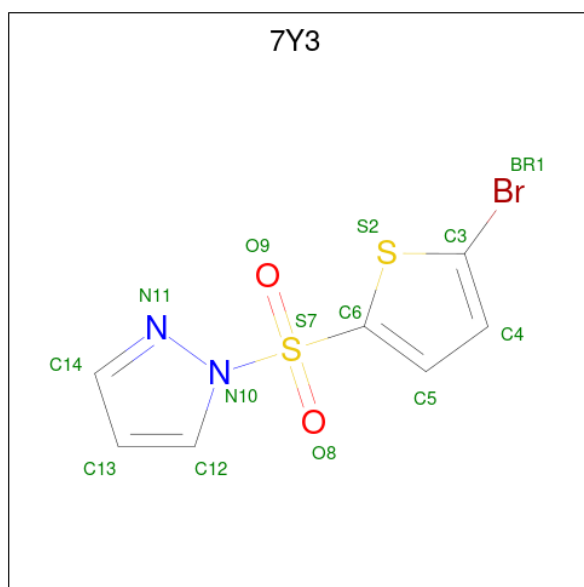
There are 4 unique types of molecules in this entry. The entry contains 7083 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 LuxR family transcriptional regulator.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	203	Total	C	N	O	S	Se	0	0	0
			1654	1045	296	306	3	4			
1	B	202	Total	C	N	O	S	Se	0	0	0
			1648	1042	295	304	3	4			
1	C	200	Total	C	N	O	S	Se	0	0	0
			1625	1029	291	298	3	4			
1	D	200	Total	C	N	O	S	Se	0	0	0
			1628	1031	291	299	3	4			

- Molecule 2 is 1-(5-bromanylthiophen-2-yl)sulfonylpyrazole (CCD ID: 7Y3) (formula: $C_7H_5BrN_2O_2S_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	Br	C	N	O	S	0	0
			14	1	7	2	2	2		
2	B	1	Total	Br	C	N	O	S	0	0
			14	1	7	2	2	2		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	C	1	Total	Br	C	N	O	S	0	0
			14	1	7	2	2	2		
2	D	1	Total	Br	C	N	O	S	0	0
			14	1	7	2	2	2		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

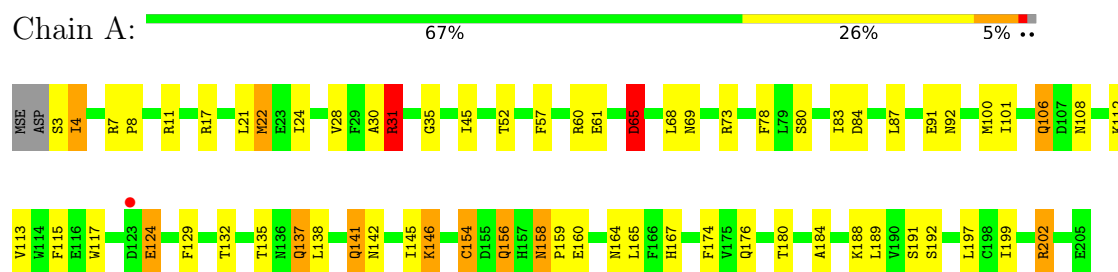
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	148	Total	O	0	0
			148	148		
4	B	116	Total	O	0	0
			116	116		
4	C	101	Total	O	0	0
			101	101		
4	D	97	Total	O	0	0
			97	97		

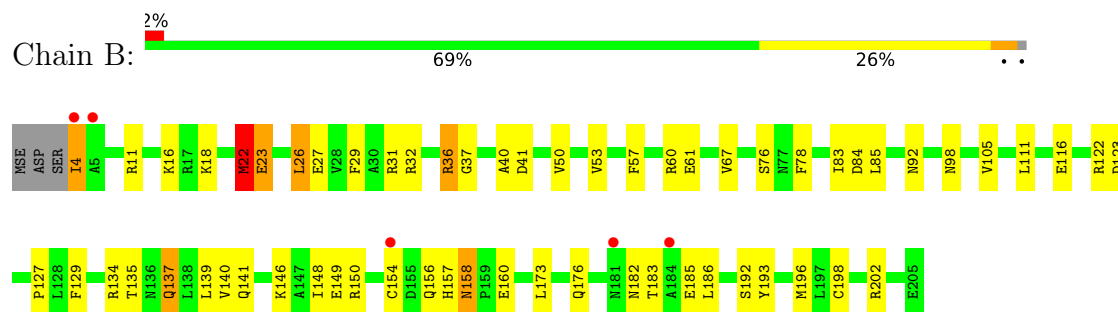
3 Residue-property plots

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.

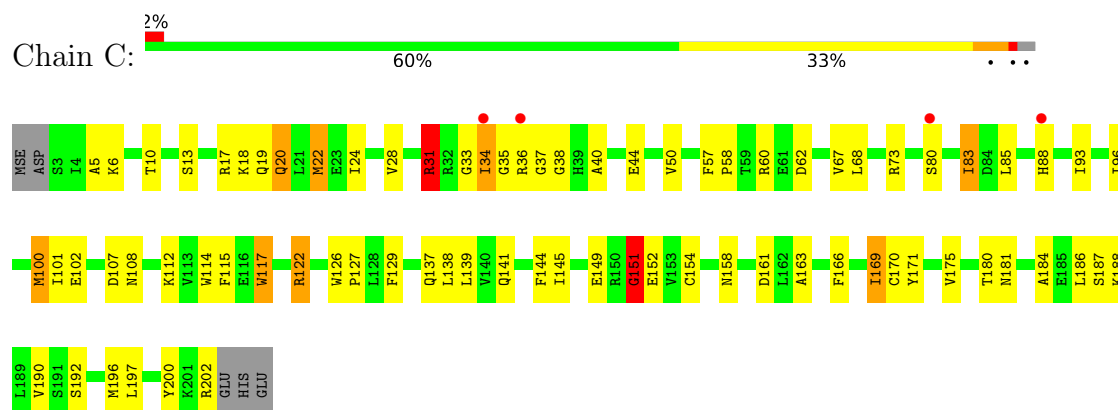
• Molecule 1: LuxR family transcriptional regulator



• Molecule 1: LuxR family transcriptional regulator

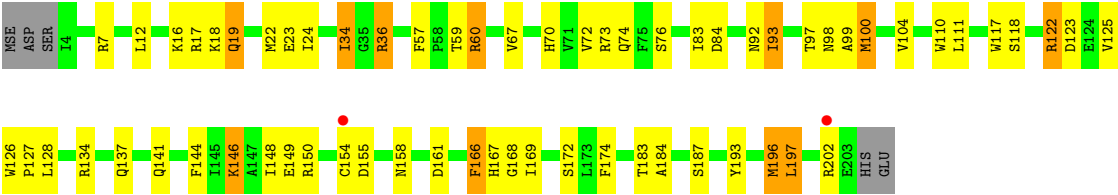


• Molecule 1: LuxR family transcriptional regulator



• Molecule 1: LuxR family transcriptional regulator





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.67Å 99.21Å 129.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 2.10 35.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (35.00-2.10) 99.8 (35.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.26 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.187 , 0.258 0.188 , 0.260	Depositor DCC
R_{free} test set	3012 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	33.8	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7083	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.09 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.3415e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 7Y3, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	2.05	45/1683 (2.7%)	1.51	9/2274 (0.4%)
1	B	1.81	25/1677 (1.5%)	1.54	13/2266 (0.6%)
1	C	1.94	42/1653 (2.5%)	1.60	15/2235 (0.7%)
1	D	1.70	19/1656 (1.1%)	1.45	8/2239 (0.4%)
All	All	1.88	131/6669 (2.0%)	1.53	45/9014 (0.5%)

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	C	0	1

All (131) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	100	MSE	N-CA	10.51	1.58	1.46
1	A	22	MSE	N-CA	10.13	1.58	1.46
1	B	98	ASN	C-O	-9.26	1.13	1.24
1	A	141	GLN	N-CA	8.91	1.57	1.46
1	A	145	ILE	N-CA	8.81	1.56	1.46
1	A	115	PHE	C-O	8.74	1.34	1.24
1	B	196	MSE	N-CA	8.68	1.57	1.46
1	C	181	ASN	CG-OD1	8.59	1.39	1.23
1	A	142	ASN	N-CA	7.98	1.56	1.46
1	D	197	LEU	C-O	7.79	1.32	1.23
1	C	73	ARG	CZ-NH1	7.66	1.43	1.32
1	A	52	THR	CA-C	7.58	1.62	1.52
1	B	122	ARG	C-O	7.41	1.32	1.24
1	B	160	GLU	C-O	7.28	1.32	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	187	SER	CA-CB	7.23	1.64	1.53
1	B	173	LEU	C-O	-7.21	1.15	1.24
1	C	80	SER	C-O	-7.13	1.15	1.24
1	A	159	PRO	C-O	7.04	1.32	1.24
1	A	191	SER	C-O	-6.95	1.16	1.24
1	C	184	ALA	CA-C	6.90	1.61	1.52
1	A	100	MSE	CA-CB	6.83	1.64	1.53
1	A	132	THR	N-CA	6.82	1.55	1.46
1	A	160	GLU	CA-C	6.76	1.61	1.52
1	B	29	PHE	N-CA	6.66	1.54	1.46
1	C	18	LYS	CA-C	6.59	1.61	1.52
1	B	111	LEU	C-O	6.51	1.31	1.24
1	B	127	PRO	N-CA	6.48	1.56	1.47
1	A	138	LEU	C-O	-6.47	1.16	1.24
1	A	21	LEU	CA-C	6.46	1.61	1.52
1	C	114	TRP	CA-CB	6.45	1.63	1.53
1	D	100	MSE	N-CA	6.45	1.54	1.46
1	A	4	ILE	N-CA	6.42	1.53	1.46
1	A	146	LYS	C-O	-6.38	1.16	1.24
1	C	197	LEU	C-O	6.35	1.31	1.23
1	D	98	ASN	N-CA	6.30	1.54	1.46
1	C	31	ARG	N-CA	6.29	1.54	1.46
1	A	137	GLN	C-O	-6.29	1.16	1.24
1	C	188	LYS	CA-C	6.27	1.60	1.52
1	C	108	ASN	CA-C	6.27	1.60	1.52
1	A	135	THR	CA-CB	6.25	1.63	1.53
1	D	70	HIS	CA-C	6.23	1.60	1.52
1	D	110	TRP	C-O	6.22	1.31	1.24
1	A	65	ASP	CB-CG	-6.15	1.36	1.52
1	A	11	ARG	C-O	-6.15	1.16	1.23
1	B	160	GLU	CA-C	6.12	1.60	1.52
1	D	183	THR	CA-C	6.12	1.60	1.52
1	A	31	ARG	C-O	-6.11	1.16	1.24
1	C	38	GLY	C-O	6.08	1.28	1.23
1	C	163	ALA	C-O	-6.06	1.17	1.24
1	D	76	SER	C-O	-6.03	1.17	1.24
1	A	113	VAL	CA-CB	6.01	1.61	1.54
1	C	171	TYR	CA-CB	6.00	1.62	1.53
1	B	198	CYS	N-CA	-5.95	1.38	1.46
1	A	167	HIS	C-O	5.91	1.30	1.24
1	C	5	ALA	CA-C	5.91	1.60	1.52
1	C	18	LYS	N-CA	5.87	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	192	SER	N-CA	5.86	1.53	1.46
1	B	158	ASN	CB-CG	-5.84	1.37	1.52
1	A	142	ASN	CA-C	-5.83	1.44	1.52
1	A	154	CYS	C-O	5.83	1.30	1.23
1	C	187	SER	N-CA	5.83	1.53	1.46
1	A	138	LEU	CA-CB	5.82	1.62	1.53
1	B	76	SER	CA-C	5.79	1.60	1.52
1	C	57	PHE	CA-C	5.78	1.58	1.52
1	D	174	PHE	C-O	5.76	1.30	1.24
1	A	87	LEU	C-O	-5.75	1.16	1.23
1	C	58	PRO	C-O	-5.75	1.16	1.24
1	C	139	LEU	CA-C	5.75	1.60	1.52
1	D	99	ALA	CA-C	5.75	1.60	1.52
1	C	83	ILE	CA-C	5.74	1.59	1.52
1	D	168	GLY	N-CA	5.74	1.52	1.45
1	C	37	GLY	N-CA	5.71	1.49	1.44
1	D	72	VAL	N-CA	5.69	1.53	1.46
1	C	28	VAL	CA-CB	5.69	1.61	1.54
1	D	73	ARG	C-O	-5.66	1.17	1.24
1	C	68	LEU	C-O	5.62	1.30	1.24
1	C	187	SER	CA-C	-5.62	1.45	1.52
1	A	101	ILE	N-CA	-5.59	1.40	1.46
1	A	28	VAL	CA-C	5.58	1.59	1.52
1	A	197	LEU	N-CA	5.57	1.53	1.46
1	C	40	ALA	C-O	5.56	1.30	1.24
1	C	24	ILE	CA-CB	5.55	1.60	1.54
1	B	193	TYR	CA-C	-5.53	1.45	1.52
1	A	113	VAL	C-O	5.53	1.30	1.24
1	D	196	MSE	N-CA	5.53	1.53	1.46
1	A	80	SER	C-O	-5.51	1.17	1.24
1	C	44	GLU	C-O	-5.51	1.17	1.24
1	B	122	ARG	N-CA	5.50	1.53	1.46
1	D	187	SER	CA-CB	5.47	1.61	1.53
1	B	148	ILE	N-CA	5.44	1.52	1.46
1	B	53	VAL	C-O	-5.44	1.18	1.24
1	A	199	ILE	CA-C	5.42	1.60	1.52
1	A	174	PHE	C-O	5.41	1.30	1.24
1	C	50	VAL	N-CA	-5.41	1.40	1.46
1	B	11	ARG	CA-C	-5.41	1.45	1.52
1	C	101	ILE	N-CA	-5.40	1.40	1.46
1	D	74	GLN	N-CA	5.37	1.52	1.46
1	C	62	ASP	CA-C	5.35	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	180	THR	N-CA	5.35	1.52	1.45
1	B	61	GLU	CA-C	5.34	1.59	1.52
1	A	8	PRO	N-CA	5.33	1.53	1.47
1	B	137	GLN	N-CA	5.33	1.52	1.46
1	A	189	LEU	CA-C	5.31	1.59	1.52
1	C	161	ASP	N-CA	-5.26	1.39	1.46
1	B	149	GLU	C-O	-5.25	1.17	1.24
1	C	117	TRP	C-O	5.24	1.30	1.24
1	A	17	ARG	N-CA	-5.24	1.39	1.46
1	C	20	GLN	C-O	5.21	1.30	1.24
1	D	150	ARG	N-CA	5.21	1.52	1.46
1	C	190	VAL	C-O	5.18	1.30	1.24
1	C	144	PHE	CA-C	5.17	1.59	1.52
1	D	83	ILE	N-CA	-5.17	1.40	1.46
1	A	83	ILE	CA-CB	-5.16	1.48	1.54
1	A	137	GLN	C-N	-5.15	1.27	1.33
1	C	115	PHE	CA-CB	-5.15	1.45	1.53
1	A	22	MSE	C-O	-5.14	1.18	1.24
1	D	184	ALA	N-CA	-5.13	1.40	1.46
1	A	57	PHE	C-O	-5.12	1.18	1.24
1	A	68	LEU	N-CA	5.12	1.52	1.46
1	B	57	PHE	N-CA	5.11	1.52	1.46
1	A	78	PHE	N-CA	-5.11	1.40	1.46
1	D	93	ILE	CA-CB	5.09	1.60	1.54
1	A	21	LEU	C-O	5.08	1.30	1.24
1	C	192	SER	CA-C	5.05	1.59	1.52
1	B	78	PHE	CA-C	5.05	1.59	1.52
1	B	18	LYS	N-CA	-5.04	1.40	1.46
1	B	85	LEU	N-CA	-5.04	1.39	1.46
1	C	122	ARG	N-CA	5.02	1.52	1.46
1	C	112	LYS	N-CA	-5.01	1.40	1.46
1	B	129	PHE	CA-C	-5.00	1.46	1.52
1	A	45	ILE	CA-CB	5.00	1.61	1.54

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	175	VAL	N-CA-C	-10.11	101.02	110.53
1	C	40	ALA	N-CA-C	7.91	119.90	111.28
1	C	33	GLY	CA-C-O	7.19	126.89	122.22
1	A	17	ARG	N-CA-C	-7.00	103.08	111.69
1	B	22	MSE	N-CA-CB	-6.77	100.03	109.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	ASN	N-CA-C	-6.61	101.73	109.93
1	B	158	ASN	N-CA-CB	-6.58	100.86	110.14
1	B	123	ASP	N-CA-C	6.56	120.87	112.34
1	B	23	GLU	N-CA-C	6.40	119.08	111.33
1	C	151	GLY	N-CA-C	6.39	121.49	114.40
1	D	123	ASP	N-CA-C	6.29	120.51	112.34
1	A	164	ASN	N-CA-C	6.12	118.03	111.36
1	D	144	PHE	N-CA-C	6.11	118.73	111.71
1	C	158	ASN	N-CA-CB	-6.10	101.29	110.32
1	A	138	LEU	N-CA-CB	-6.04	101.23	110.12
1	C	36	ARG	N-CA-C	5.82	119.85	112.87
1	C	186	LEU	N-CA-C	-5.80	104.55	111.69
1	C	101	ILE	N-CA-C	5.73	116.38	110.36
1	D	134	ARG	N-CA-C	5.69	117.94	111.11
1	D	104	VAL	N-CA-C	-5.66	103.85	111.44
1	B	16	LYS	N-CA-C	5.66	117.45	111.28
1	C	102	GLU	N-CA-C	-5.64	105.13	111.28
1	B	158	ASN	CB-CA-C	-5.63	100.99	109.26
1	C	33	GLY	N-CA-C	5.61	117.28	111.95
1	B	134	ARG	NE-CZ-NH1	-5.45	116.05	121.50
1	A	4	ILE	N-CA-CB	5.43	116.85	110.82
1	D	166	PHE	N-CA-C	-5.36	105.52	111.36
1	B	192	SER	CB-CA-C	-5.36	101.57	110.68
1	B	41	ASP	N-CA-C	-5.31	105.40	111.14
1	A	80	SER	CA-CB-OG	-5.25	100.61	111.10
1	B	140	VAL	N-CA-C	-5.23	105.44	110.72
1	A	156	GLN	N-CA-C	-5.19	106.73	113.16
1	A	91	GLU	N-CA-C	5.16	116.91	111.28
1	D	172	SER	N-CA-C	-5.15	105.75	111.36
1	C	13	SER	CA-C-N	-5.15	113.62	119.28
1	C	13	SER	C-N-CA	-5.15	113.62	119.28
1	C	169	ILE	N-CA-C	-5.12	105.42	111.00
1	C	187	SER	CA-CB-OG	-5.12	100.85	111.10
1	D	150	ARG	CB-CG-CD	-5.10	99.57	111.30
1	A	132	THR	CA-CB-OG1	-5.09	101.96	109.60
1	B	116	GLU	CA-CB-CG	-5.07	103.96	114.10
1	C	22	MSE	CG-SE-CE	-5.03	87.85	98.92
1	D	97	THR	OG1-CB-CG2	-5.03	99.24	109.30
1	B	185	GLU	CA-C-N	5.02	127.42	120.29
1	B	185	GLU	C-N-CA	5.02	127.42	120.29

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	151	GLY	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1654	0	1632	26	0
1	B	1648	0	1627	24	0
1	C	1625	0	1612	28	0
1	D	1628	0	1613	38	0
2	A	14	0	0	0	0
2	B	14	0	0	0	0
2	C	14	0	0	1	0
2	D	14	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	148	0	0	3	0
4	B	116	0	0	3	0
4	C	101	0	0	0	0
4	D	97	0	0	2	0
All	All	7083	0	6484	108	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (108) 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:157:HIS:HB3	1:C:196:MSE:HE2	1.43	0.98
1:C:151:GLY:HA3	1:C:202:ARG:HE	1.27	0.94
1:D:122:ARG:HG3	1:D:122:ARG:HH11	1.31	0.94
1:D:137:GLN:HE21	1:D:141:GLN:NE2	1.70	0.90
1:D:137:GLN:HE21	1:D:141:GLN:HE21	0.90	0.89
1:C:151:GLY:HA3	1:C:202:ARG:NE	1.87	0.88
1:C:34:ILE:H	1:C:34:ILE:HD12	1.43	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:GLN:HE21	1:A:141:GLN:HE21	1.24	0.82
1:D:60:ARG:HH11	1:D:60:ARG:CG	1.93	0.82
1:A:84:ASP:H	1:A:92:ASN:HD21	1.31	0.78
1:B:36:ARG:HH12	1:B:40:ALA:H	1.29	0.77
1:D:137:GLN:NE2	1:D:141:GLN:HE21	1.76	0.77
1:B:202:ARG:HD2	1:D:149:GLU:OE1	1.88	0.73
1:D:36:ARG:HH11	1:D:36:ARG:HG2	1.56	0.71
1:B:202:ARG:NH1	1:D:146:LYS:HE3	2.05	0.71
1:A:84:ASP:H	1:A:92:ASN:ND2	1.89	0.71
1:B:137:GLN:HE21	1:B:141:GLN:HE21	1.41	0.68
1:B:154:CYS:SG	1:B:156:GLN:HG2	2.34	0.68
1:D:122:ARG:HG3	1:D:122:ARG:NH1	2.05	0.66
1:A:69:ASN:O	1:A:73:ARG:HG3	1.97	0.64
4:A:743:HOH:O	1:D:167:HIS:HD2	1.80	0.64
1:C:17:ARG:HH11	1:C:20:GLN:HE22	1.45	0.63
1:A:176:GLN:HE21	1:A:180:THR:HG22	1.62	0.63
1:B:139:LEU:C	1:B:139:LEU:HD23	2.24	0.62
1:B:4:ILE:HG13	1:B:32:ARG:NH2	2.14	0.62
1:D:202:ARG:HD3	4:D:773:HOH:O	1.99	0.62
1:C:170:CYS:SG	2:C:601:7Y3:BR1	3.12	0.62
1:C:137:GLN:HE21	1:C:141:GLN:HE21	1.46	0.61
1:D:60:ARG:HH11	1:D:60:ARG:HG2	1.65	0.61
1:D:60:ARG:HH11	1:D:60:ARG:HG3	1.64	0.61
1:A:61:GLU:O	1:A:65:ASP:HB2	2.02	0.60
1:D:84:ASP:O	1:D:92:ASN:ND2	2.35	0.60
1:C:145:ILE:O	1:C:149:GLU:HG3	2.03	0.58
1:C:93:ILE:HG23	1:C:166:PHE:CE1	2.38	0.57
1:D:100:MSE:HG2	1:D:111:LEU:HD21	1.86	0.57
1:C:151:GLY:CA	1:C:202:ARG:HE	2.10	0.57
1:B:202:ARG:HH12	1:D:146:LYS:HE3	1.68	0.56
1:A:184:ALA:O	1:A:188:LYS:HD3	2.05	0.56
1:C:31:ARG:NH2	1:C:107:ASP:OD1	2.38	0.55
1:D:19:GLN:NE2	1:D:23:GLU:OE2	2.38	0.55
1:A:154:CYS:SG	1:A:156:GLN:HG2	2.47	0.55
1:B:37:GLY:HA2	1:B:60:ARG:HG3	1.87	0.55
1:A:61:GLU:H	1:A:61:GLU:CD	2.14	0.54
1:B:31:ARG:HD2	4:B:805:HOH:O	2.07	0.54
1:C:83:ILE:HG12	1:C:96:ILE:HD11	1.90	0.54
1:A:73:ARG:NH2	4:A:704:HOH:O	2.40	0.54
1:D:60:ARG:CG	1:D:60:ARG:NH1	2.60	0.54
1:D:60:ARG:HG2	1:D:60:ARG:NH1	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:ARG:HG3	1:D:24:ILE:HD11	1.89	0.54
1:C:17:ARG:HH11	1:C:20:GLN:NE2	2.06	0.54
1:A:3:SER:N	1:A:31:ARG:NH2	2.56	0.53
1:A:137:GLN:HE21	1:A:141:GLN:NE2	2.01	0.53
1:A:176:GLN:HE21	1:A:180:THR:CG2	2.22	0.52
1:C:34:ILE:H	1:C:34:ILE:CD1	2.11	0.52
1:A:202:ARG:HD3	1:C:149:GLU:OE2	2.10	0.52
1:A:165:LEU:HD22	1:D:196:MSE:HE3	1.92	0.51
1:A:106:GLN:HE21	1:A:108:ASN:HD21	1.59	0.51
1:A:4:ILE:H	1:A:31:ARG:HH21	1.58	0.50
1:B:84:ASP:H	1:B:92:ASN:HD21	1.58	0.50
1:C:88:HIS:CG	1:C:152:GLU:OE2	2.65	0.49
4:B:745:HOH:O	1:D:146:LYS:HD2	2.11	0.49
1:B:4:ILE:HD13	1:B:27:GLU:HG2	1.95	0.48
1:B:22:MSE:HG3	1:B:23:GLU:N	2.28	0.48
1:A:35:GLY:CA	1:A:60:ARG:HH22	2.27	0.48
1:B:22:MSE:C	1:B:22:MSE:SE	3.07	0.47
1:D:193:TYR:HA	1:D:196:MSE:CE	2.44	0.47
1:A:84:ASP:N	1:A:92:ASN:HD21	2.06	0.47
1:B:139:LEU:HD23	1:B:139:LEU:O	2.12	0.47
1:B:92:ASN:ND2	4:B:707:HOH:O	2.46	0.47
1:D:169:ILE:HD13	1:D:197:LEU:HD11	1.96	0.47
1:C:22:MSE:SE	1:C:67:VAL:HG22	2.64	0.47
1:A:7:ARG:HG3	1:A:24:ILE:HD11	1.98	0.46
1:D:12:LEU:HD12	1:D:17:ARG:CZ	2.45	0.46
1:A:22:MSE:HE2	1:A:22:MSE:HB2	1.67	0.46
1:A:92:ASN:ND2	4:A:712:HOH:O	2.49	0.46
1:D:158:ASN:HD22	1:D:161:ASP:CG	2.24	0.46
1:C:126:TRP:CG	1:C:127:PRO:HD3	2.50	0.46
1:D:193:TYR:HA	1:D:196:MSE:HE3	1.97	0.46
1:D:93:ILE:HG23	1:D:166:PHE:CE1	2.50	0.45
1:A:117:TRP:CD1	1:A:129:PHE:HB2	2.52	0.45
1:D:148:ILE:HG23	1:D:155:ASP:HA	1.98	0.45
1:A:124:GLU:H	1:A:124:GLU:CD	2.25	0.45
1:B:4:ILE:HG12	1:B:31:ARG:HD3	1.99	0.45
1:B:157:HIS:CB	1:C:196:MSE:HE2	2.30	0.45
1:C:31:ARG:HA	1:C:31:ARG:HD3	1.75	0.45
1:B:26:LEU:HD12	1:B:67:VAL:HG13	1.99	0.44
1:A:106:GLN:NE2	1:A:108:ASN:HD21	2.16	0.43
1:D:117:TRP:CZ3	1:D:125:VAL:CG1	3.02	0.43
1:C:35:GLY:O	1:C:60:ARG:NH2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:ILE:HD12	1:B:139:LEU:HD21	2.00	0.42
1:C:126:TRP:CD2	1:C:127:PRO:HD3	2.54	0.42
1:D:126:TRP:N	1:D:127:PRO:CD	2.82	0.42
1:B:137:GLN:HE21	1:B:141:GLN:NE2	2.11	0.42
1:B:84:ASP:H	1:B:92:ASN:ND2	2.18	0.42
1:C:202:ARG:HD3	1:C:202:ARG:HA	1.80	0.42
1:C:35:GLY:C	1:C:60:ARG:HH22	2.27	0.42
1:C:200:TYR:OH	1:D:155:ASP:OD2	2.32	0.41
1:D:118:SER:OG	1:D:167:HIS:CE1	2.73	0.41
1:C:100:MSE:SE	1:C:100:MSE:C	3.13	0.41
1:A:30:ALA:O	1:A:112:LYS:HE2	2.20	0.41
1:B:40:ALA:HA	1:B:50:VAL:HG22	2.03	0.41
1:D:154:CYS:HB2	4:D:752:HOH:O	2.20	0.41
1:D:117:TRP:CZ3	1:D:125:VAL:HG13	2.55	0.41
1:C:169:ILE:HG21	1:C:169:ILE:HD13	1.83	0.41
1:D:18:LYS:HE3	1:D:57:PHE:CE1	2.56	0.41
1:D:22:MSE:SE	1:D:67:VAL:HG22	2.71	0.41
1:D:34:ILE:HG12	1:D:117:TRP:CD1	2.56	0.41
1:C:117:TRP:CD1	1:C:129:PHE:HB2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	201/205 (98%)	198 (98%)	3 (2%)	0	100	100
1	B	200/205 (98%)	195 (98%)	4 (2%)	1 (0%)	24	22
1	C	198/205 (97%)	193 (98%)	5 (2%)	0	100	100
1	D	198/205 (97%)	194 (98%)	4 (2%)	0	100	100
All	All	797/820 (97%)	780 (98%)	16 (2%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	182	ASN

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	182/179 (102%)	175 (96%)	7 (4%)	29	32
1	B	181/179 (101%)	169 (93%)	12 (7%)	15	13
1	C	179/179 (100%)	170 (95%)	9 (5%)	22	22
1	D	179/179 (100%)	170 (95%)	9 (5%)	22	22
All	All	721/716 (101%)	684 (95%)	37 (5%)	21	21

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ARG
1	A	65	ASP
1	A	106	GLN
1	A	124	GLU
1	A	146	LYS
1	A	158	ASN
1	A	202	ARG
1	B	4	ILE
1	B	22	MSE
1	B	26	LEU
1	B	36	ARG
1	B	105	VAL
1	B	135	THR
1	B	146	LYS
1	B	150	ARG
1	B	158	ASN
1	B	176	GLN
1	B	183	THR
1	B	186	LEU

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Mol	Chain	Res	Type
1	C	6	LYS
1	C	10	THR
1	C	19	GLN
1	C	31	ARG
1	C	34	ILE
1	C	85	LEU
1	C	122	ARG
1	C	138	LEU
1	C	154	CYS
1	D	16	LYS
1	D	19	GLN
1	D	34	ILE
1	D	36	ARG
1	D	59	THR
1	D	60	ARG
1	D	122	ARG
1	D	128	LEU
1	D	146	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	HIS
1	A	74	GLN
1	A	92	ASN
1	A	98	ASN
1	A	106	GLN
1	A	141	GLN
1	A	176	GLN
1	A	204	HIS
1	B	47	GLN
1	B	70	HIS
1	B	74	GLN
1	B	92	ASN
1	B	98	ASN
1	B	141	GLN
1	B	158	ASN
1	B	204	HIS
1	C	20	GLN
1	C	47	GLN
1	C	70	HIS
1	C	141	GLN

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Mol	Chain	Res	Type
1	C	176	GLN
1	D	47	GLN
1	D	141	GLN
1	D	158	ASN
1	D	164	ASN
1	D	167	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 ⓘ

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	7Y3	B	601	-	13,15,15	2.37	3 (23%)	15,22,22	3.28	9 (60%)
2	7Y3	D	601	-	13,15,15	3.89	6 (46%)	15,22,22	2.84	5 (33%)
2	7Y3	A	601	-	13,15,15	2.71	4 (30%)	15,22,22	3.02	7 (46%)
3	SO4	B	602	-	4,4,4	0.53	0	6,6,6	0.15	0
2	7Y3	C	601	-	13,15,15	3.71	4 (30%)	15,22,22	2.47	6 (40%)
3	SO4	A	602	-	4,4,4	0.42	0	6,6,6	0.87	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	7Y3	D	601	-	-	0/12/12/12	0/2/2/2
2	7Y3	B	601	-	-	0/12/12/12	0/2/2/2
2	7Y3	A	601	-	-	0/12/12/12	0/2/2/2
2	7Y3	C	601	-	-	0/12/12/12	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	7Y3	BR1-C3	11.74	2.08	1.87
2	D	601	7Y3	BR1-C3	10.22	2.05	1.87
2	D	601	7Y3	O9-S7	7.07	1.50	1.43
2	A	601	7Y3	BR1-C3	6.92	1.99	1.87
2	B	601	7Y3	BR1-C3	6.46	1.98	1.87
2	D	601	7Y3	N10-N11	4.30	1.42	1.37
2	A	601	7Y3	N10-N11	4.26	1.42	1.37
2	B	601	7Y3	N10-N11	4.18	1.42	1.37
2	A	601	7Y3	C12-C13	3.78	1.45	1.37
2	C	601	7Y3	O9-S7	3.67	1.47	1.43
2	D	601	7Y3	C4-C3	3.02	1.41	1.35
2	C	601	7Y3	N10-N11	2.95	1.40	1.37
2	C	601	7Y3	C4-C3	2.53	1.40	1.35
2	A	601	7Y3	O8-S7	2.49	1.45	1.43
2	B	601	7Y3	C12-C13	2.42	1.42	1.37
2	D	601	7Y3	C3-S2	2.16	1.76	1.72
2	D	601	7Y3	C14-N11	2.06	1.38	1.33

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	7Y3	C4-C3-S2	7.40	120.44	113.11
2	B	601	7Y3	C4-C3-S2	6.80	119.85	113.11
2	D	601	7Y3	O9-S7-N10	6.57	113.98	104.88
2	B	601	7Y3	C5-C6-S2	5.73	118.25	112.55
2	D	601	7Y3	C5-C6-S2	5.57	118.08	112.55
2	C	601	7Y3	O9-S7-O8	-5.38	111.98	119.69
2	B	601	7Y3	BR1-C3-S2	-5.09	113.23	119.68
2	A	601	7Y3	C5-C6-S2	4.81	117.33	112.55
2	C	601	7Y3	O9-S7-N10	4.78	111.51	104.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	7Y3	O9-S7-N10	4.06	110.50	104.88
2	A	601	7Y3	BR1-C3-S2	-3.84	114.81	119.68
2	A	601	7Y3	O9-S7-N10	3.59	109.85	104.88
2	D	601	7Y3	S7-N10-N11	3.48	125.34	119.95
2	D	601	7Y3	C4-C5-C6	-3.46	108.48	112.34
2	B	601	7Y3	S7-N10-N11	3.45	125.31	119.95
2	A	601	7Y3	C5-C4-C3	-3.36	107.97	111.62
2	C	601	7Y3	O8-S7-N10	3.31	109.47	104.88
2	D	601	7Y3	O9-S7-O8	-3.08	115.28	119.69
2	C	601	7Y3	C4-C3-S2	-2.62	110.51	113.11
2	A	601	7Y3	S7-N10-N11	2.62	124.01	119.95
2	B	601	7Y3	C5-C4-C3	-2.58	108.81	111.62
2	C	601	7Y3	S7-N10-N11	2.57	123.94	119.95
2	C	601	7Y3	C5-C6-S7	2.32	131.13	126.21
2	A	601	7Y3	O9-S7-O8	-2.17	116.57	119.69
2	B	601	7Y3	O9-S7-O8	-2.11	116.66	119.69
2	B	601	7Y3	C4-C5-C6	-2.07	110.02	112.34
2	B	601	7Y3	C13-C14-N11	-2.07	107.52	111.72

There are no chirality outliers.

There are no torsion outliers.

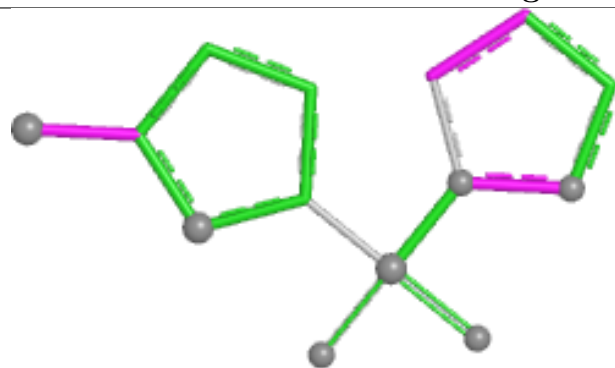
There are no ring outliers.

1 monomer is involved in 1 short contact:

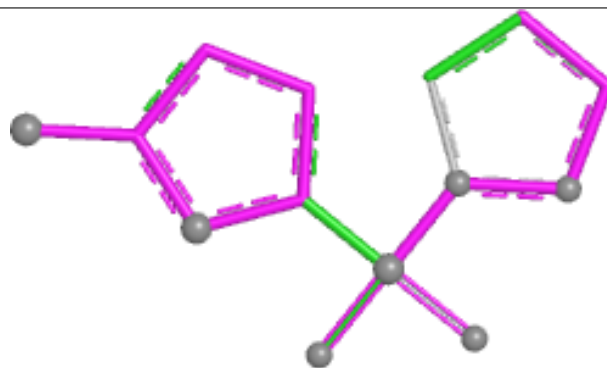
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	7Y3	1	0

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.

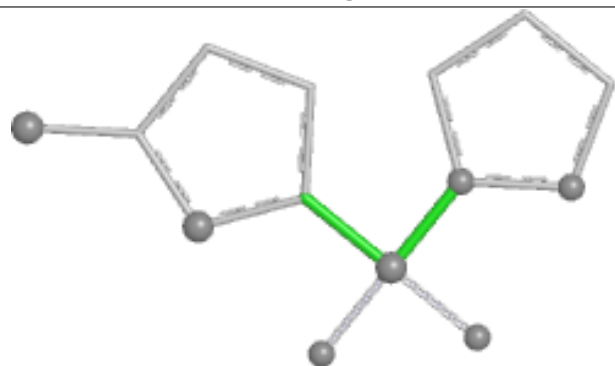
Ligand 7Y3 B 601



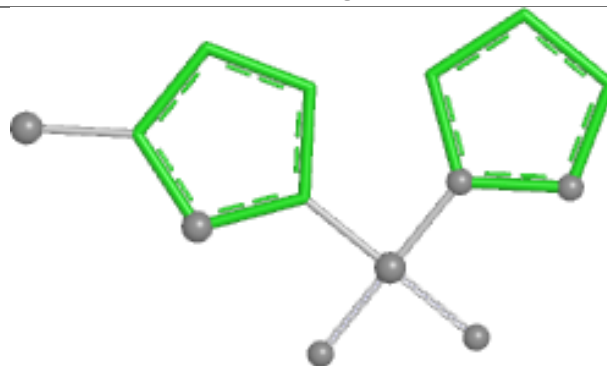
Bond lengths



Bond angles



Torsions

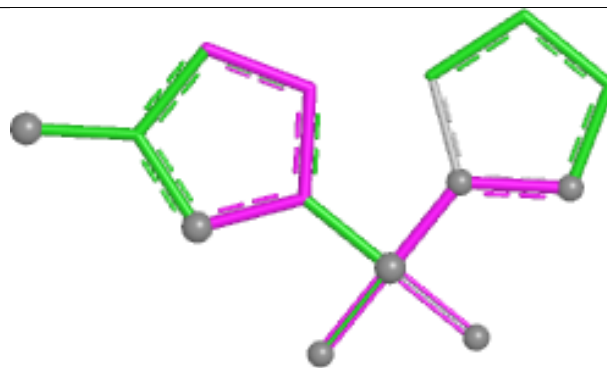


Rings

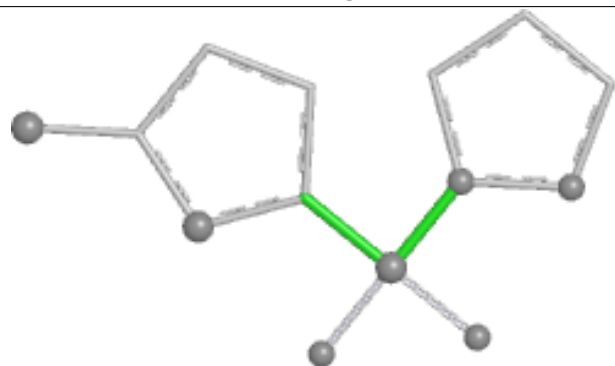
Ligand 7Y3 D 601



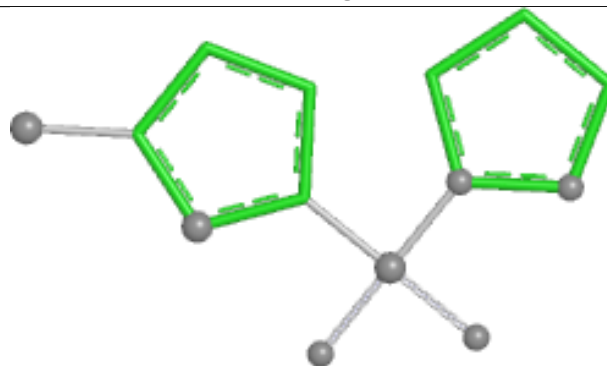
Bond lengths



Bond angles

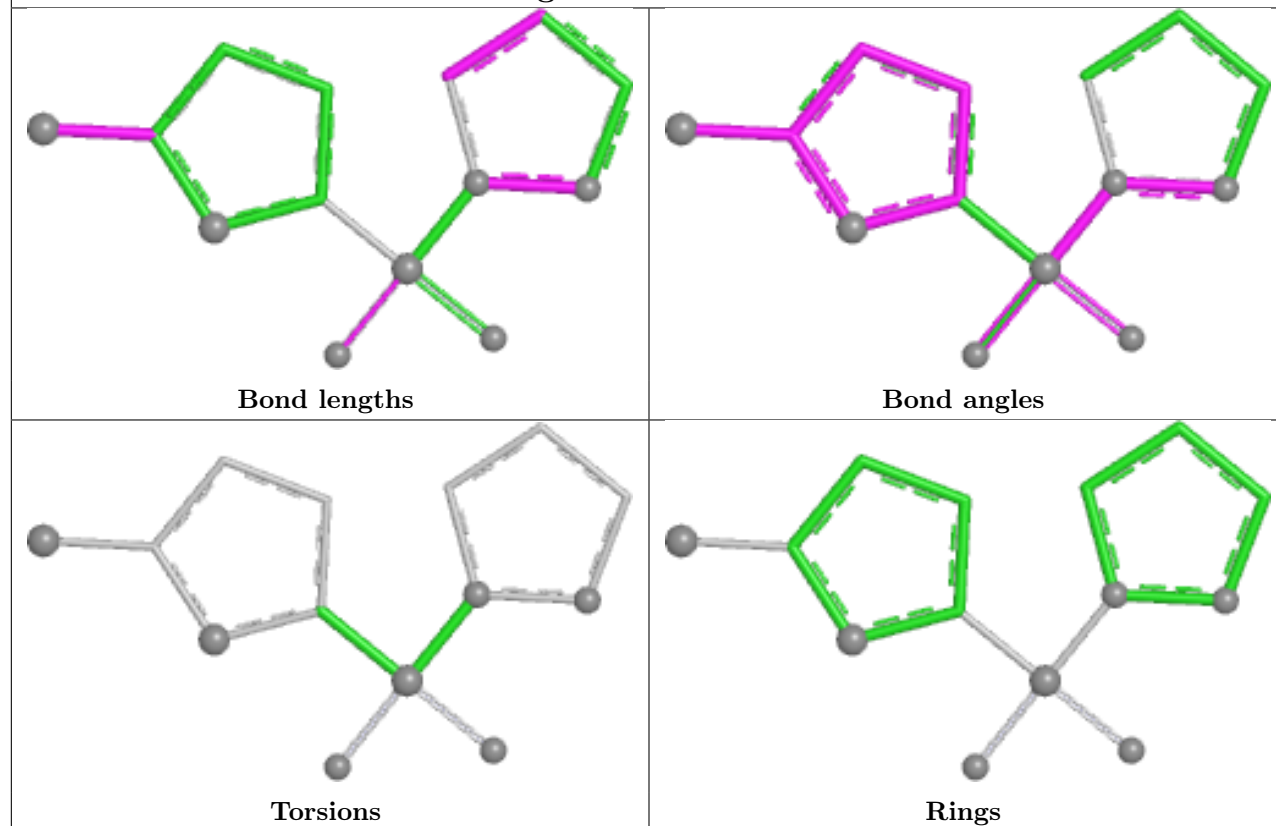


Torsions

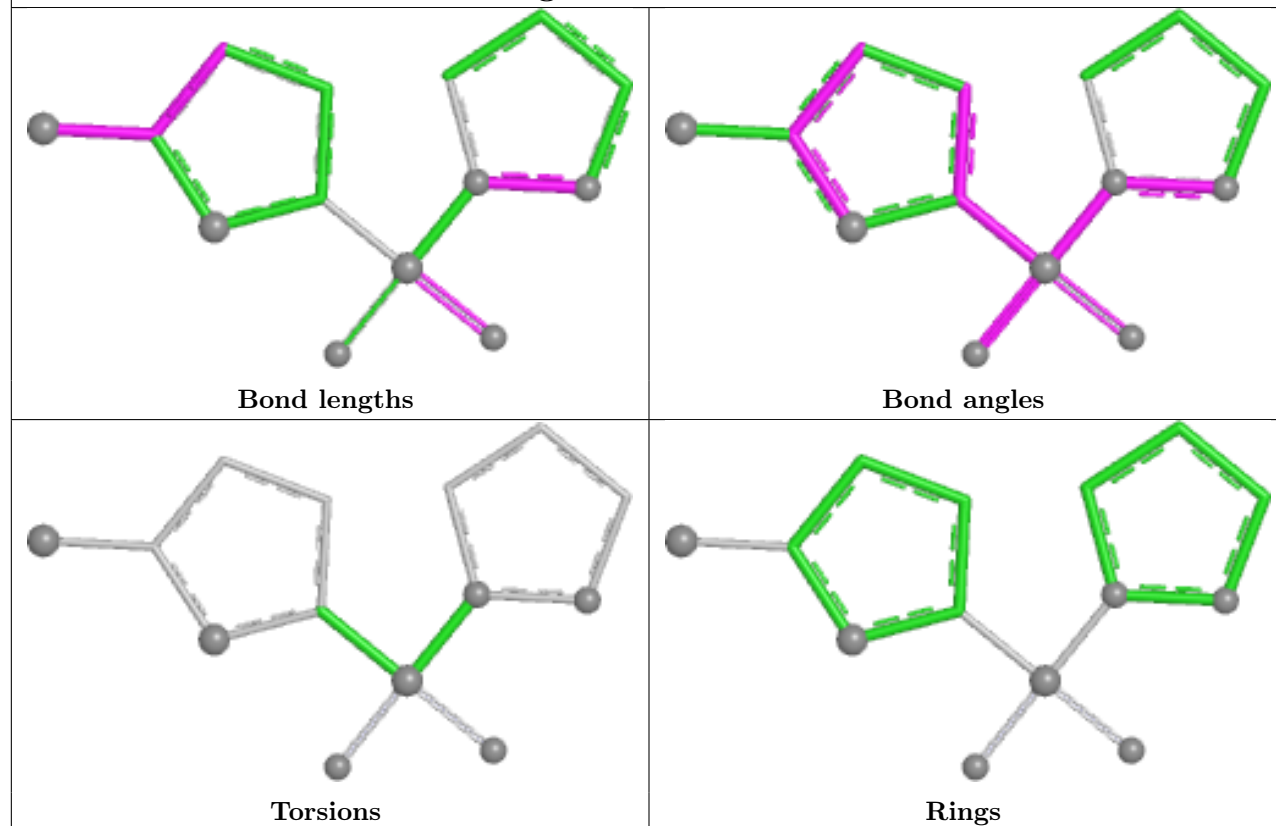


Rings

Ligand 7Y3 A 601



Ligand 7Y3 C 601



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	199/205 (97%)	-0.34	1 (0%) 87 88	21, 34, 61, 78	0
1	B	198/205 (96%)	-0.11	5 (2%) 58 61	23, 39, 66, 82	1 (0%)
1	C	196/205 (95%)	-0.02	4 (2%) 65 67	23, 41, 64, 97	2 (1%)
1	D	196/205 (95%)	-0.03	2 (1%) 79 81	25, 43, 71, 86	2 (1%)
All	All	789/820 (96%)	-0.13	12 (1%) 72 74	21, 39, 66, 97	5 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	80	SER	3.2
1	B	154	CYS	3.0
1	D	154	CYS	2.8
1	A	123	ASP	2.5
1	B	4	ILE	2.4
1	C	88	HIS	2.4
1	B	184	ALA	2.3
1	D	202	ARG	2.1
1	B	5	ALA	2.1
1	C	36	ARG	2.0
1	C	34	ILE	2.0
1	B	181	ASN	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 ⓘ

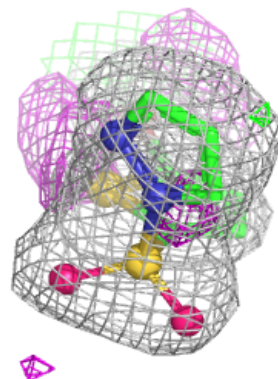
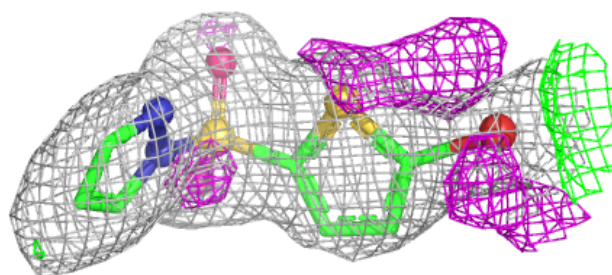
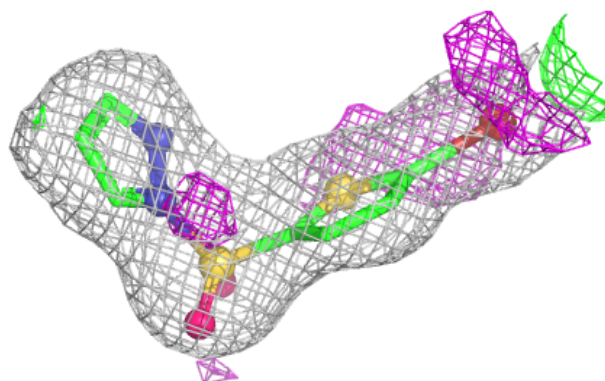
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	B	602	5/5	0.68	0.11	101,106,110,121	0
2	7Y3	C	601	14/14	0.85	0.11	49,59,72,117	0
2	7Y3	D	601	14/14	0.89	0.09	41,45,63,129	0
2	7Y3	B	601	14/14	0.92	0.10	32,41,50,104	0
2	7Y3	A	601	14/14	0.93	0.09	28,35,46,99	0
3	SO4	A	602	5/5	0.97	0.07	38,39,46,48	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.

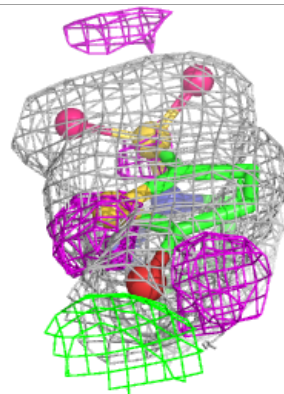
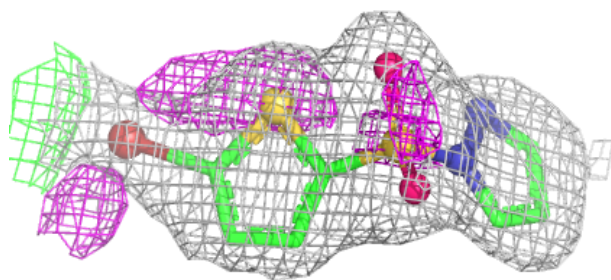
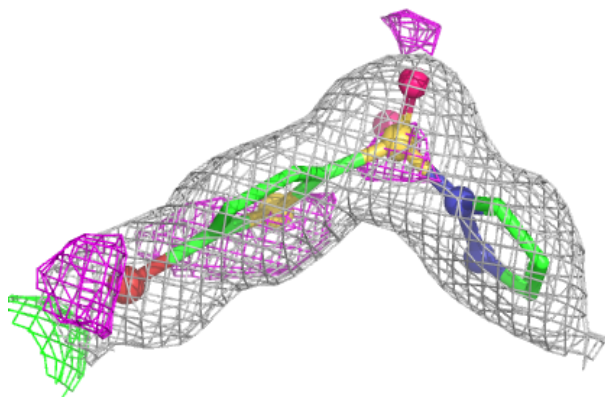
Electron density around 7Y3 C 601:

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

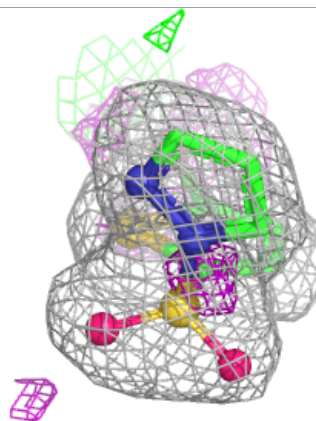
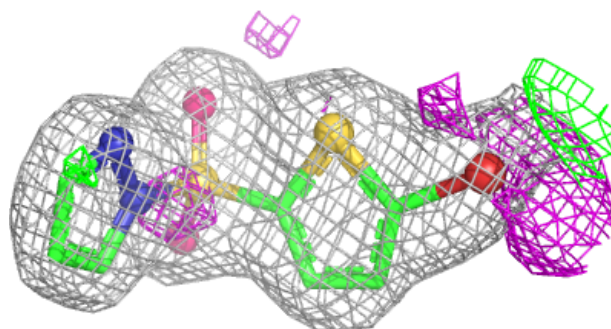
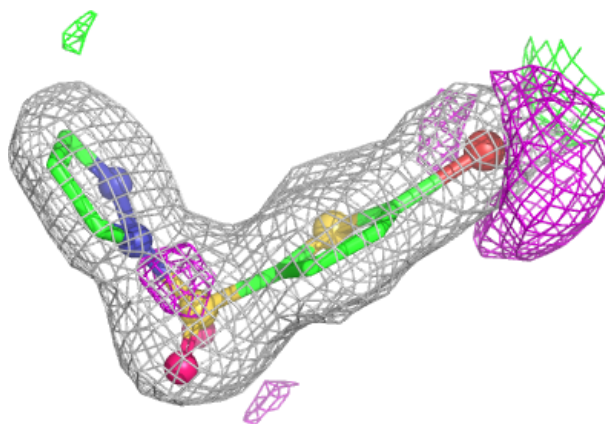


Electron density around 7Y3 D 601:

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

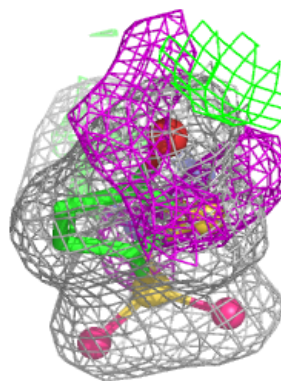
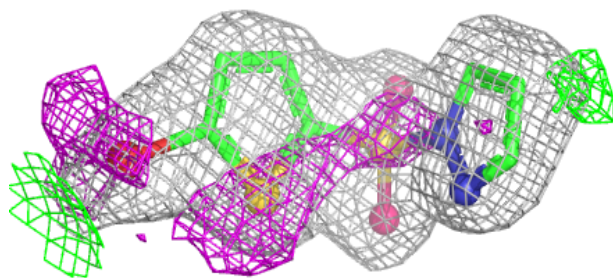
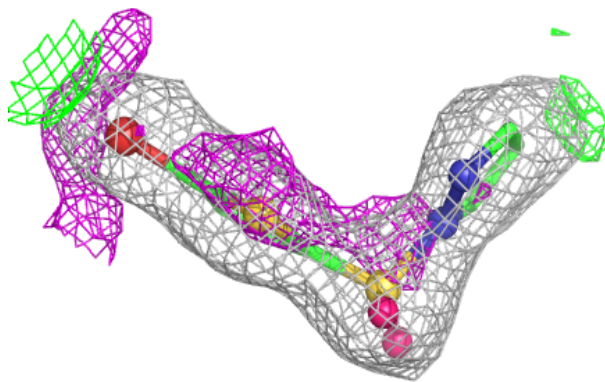
**Electron density around 7Y3 B 601:**

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



Electron density around 7Y3 A 601:

$2mF_o - DF_c$ (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.