Full wwPDB X-ray Structure Validation Report (i)

Sep 26, 2023 – 11:10 AM EDT

PDB ID	:	6C0R
Title	:	Crystal structure of HIV-1 K103N/Y181C mutant reverse transcriptase in complex with non-nucleoside inhibitor 25a
Authors	:	Yang, Y.; Nguyen, L.A.; Smithline, Z.B.; Steitz, T.A.
Deposited on	:	2018-01-02
Resolution	:	2.05 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:

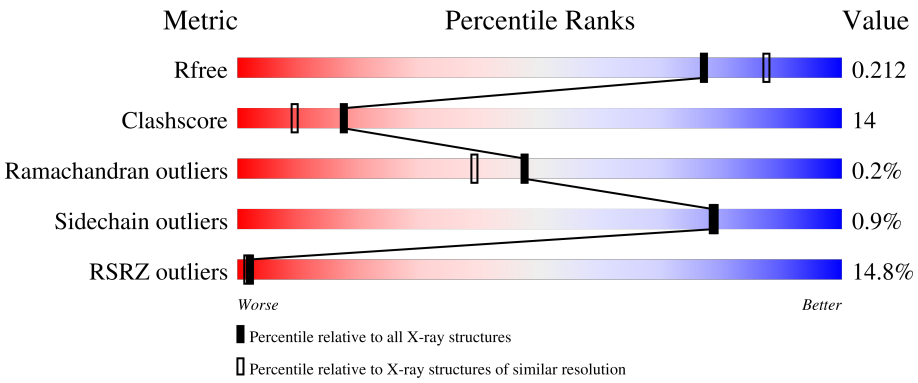
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	557	16% 73% 27%
2	B	428	13% 75% 20%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MG	A	602	-	-	-	X
6	EDO	A	612	-	-	X	-
6	EDO	A	620	-	-	-	X
6	EDO	A	623	-	-	-	X
6	EDO	A	624	-	-	X	-
6	EDO	A	627	-	-	X	-
6	EDO	A	629	-	-	-	X
6	EDO	B	512	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 8899 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 Reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	556	4586	2966	764	847	9	0	9	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP P03366
A	0	VAL	-	expression tag	UNP P03366
A	103	ASN	LYS	engineered mutation	UNP P03366
A	172	ALA	LYS	engineered mutation	UNP P03366
A	173	ALA	LYS	engineered mutation	UNP P03366
A	181	CYS	TYR	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366

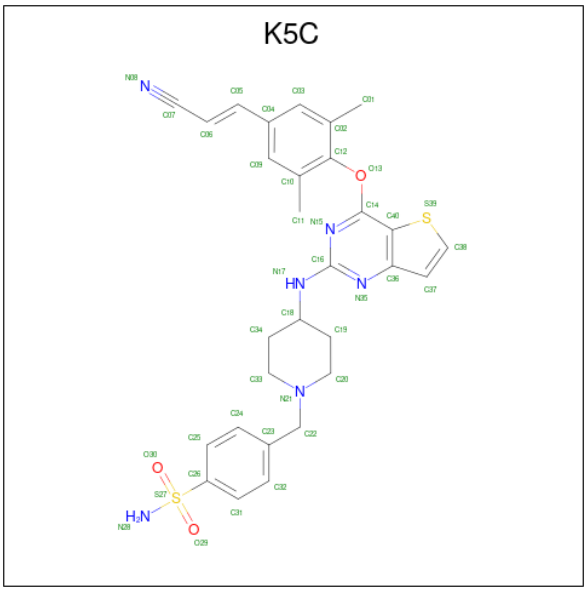
- Molecule 2 is a protein called Reverse transcriptase p51 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	412	3465	2258	572	628	7	0	7	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is 4-({4-[(4-{4-[(E)-2-cyanoethenyl]-2,6-dimethylphenoxy}thieno[3,2-d]pyrimidin-2-yl)amino]piperidin-1-yl}methyl)benzene-1-sulfonamide (three-letter code: K5C) (formula: $C_{29}H_{30}N_6O_3S_2$) (labeled as "Ligand of Interest" by depositor).

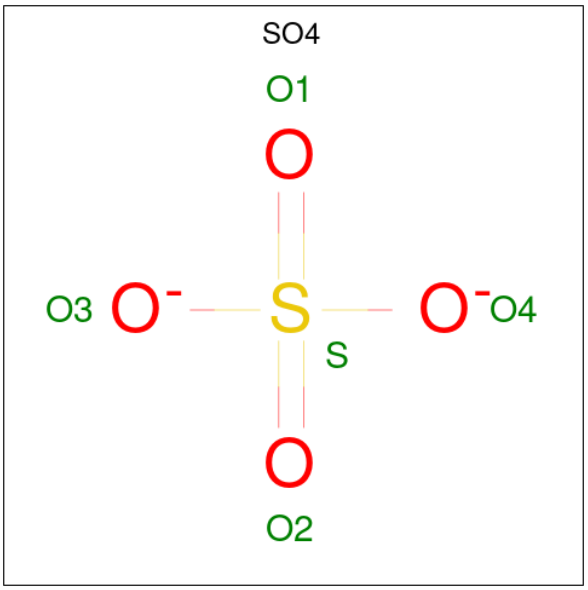


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	40	29	6	3	2	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

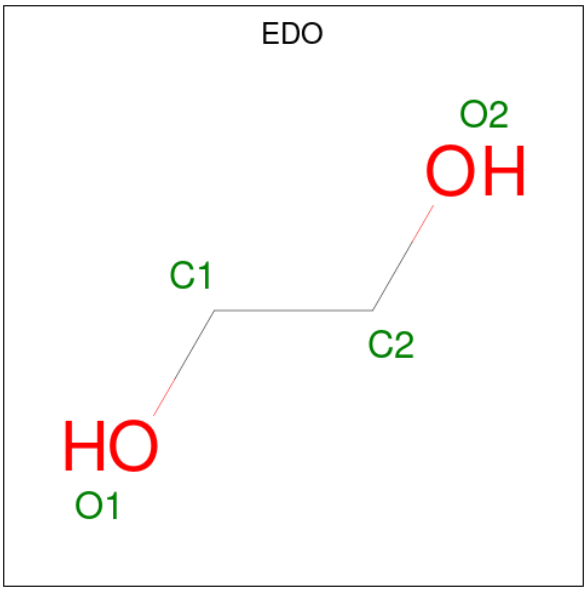
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	A	1	1	1	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	4	2	2	0	0
			Total	C	O		
6	A	1	4	2	2	0	0
			Total	C	O		
6	A	1	4	2	2	0	0
			Total	C	O		
6	A	1	4	2	2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	4	2	2	0	0
6	A	1	4	2	2	0	0
6	A	1	4	2	2	0	0
6	A	1	4	2	2	0	0
6	A	1	4	2	2	0	0
6	A	1	4	2	2	0	0
6	A	1	4	2	2	0	0
6	A	1	4	2	2	0	0
6	A	1	4	2	2	0	0
6	A	1	4	2	2	0	0
6	A	1	4	2	2	0	0
6	A	1	4	2	2	0	0
6	A	1	4	2	2	0	0
6	A	1	4	2	2	0	0
6	A	1	4	2	2	0	0
6	A	1	4	2	2	0	0
6	A	1	4	2	2	0	0
6	A	1	4	2	2	0	0
6	B	1	4	2	2	0	0
6	B	1	4	2	2	0	0
6	B	1	4	2	2	0	0

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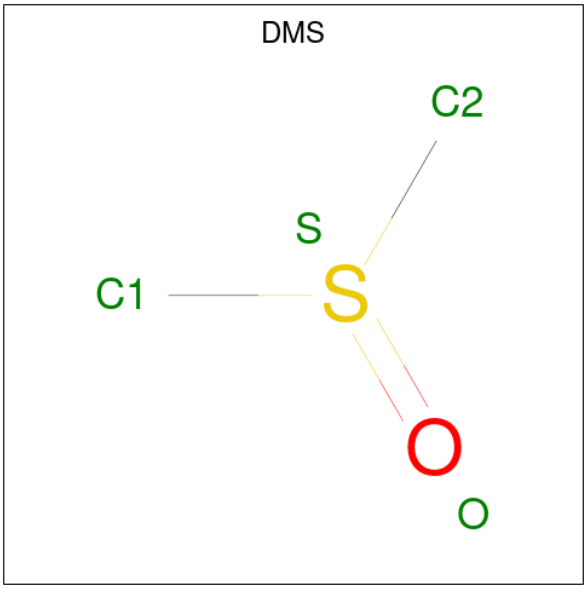
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
6	B	1	4	2	2		0	0
			Total	C	O			
6	B	1	4	2	2		0	0
			Total	C	O			
6	B	1	4	2	2		0	0
			Total	C	O			
6	B	1	4	2	2		0	0
			Total	C	O			
6	B	1	4	2	2		0	0
			Total	C	O			
6	B	1	4	2	2		0	0

- Molecule 7 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
7	B	1	4	2	1	1	0	0

- Molecule 8 is water.

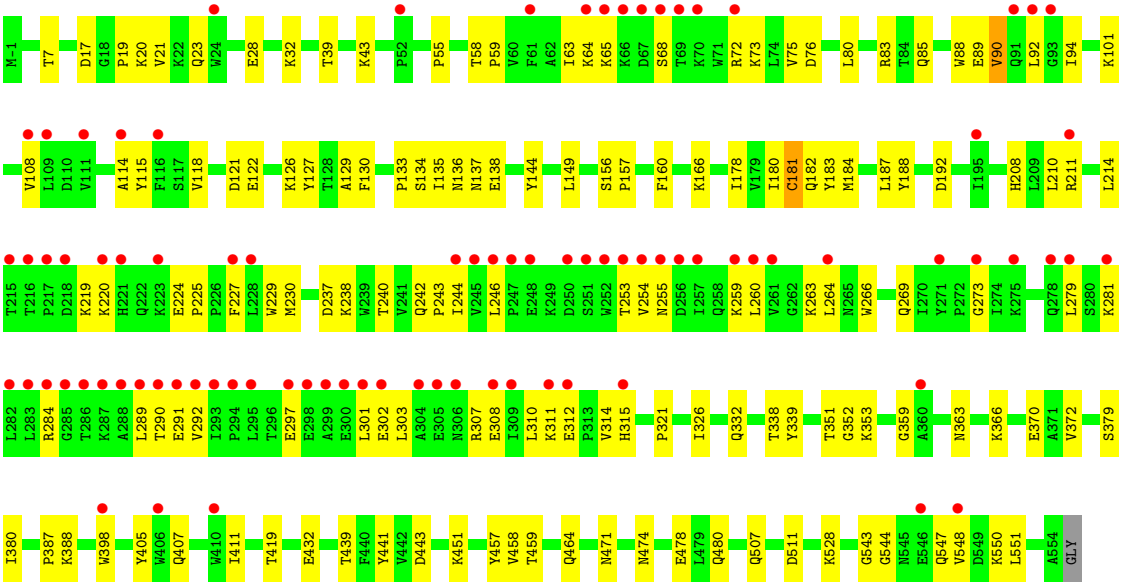
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	356	356	356	0	0
			Total	O		
8	B	283	283	283	0	0

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.

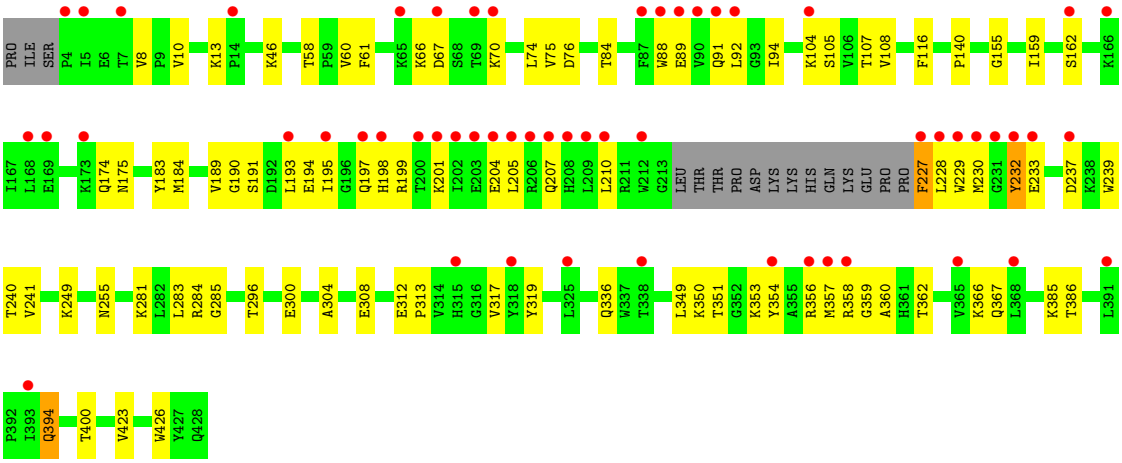
• Molecule 1: Reverse transcriptase/ribonuclease H

Chain A:



• Molecule 2: Reverse transcriptase p51 subunit

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	162.82Å 73.06Å 109.08Å 90.00° 100.47° 90.00°	Depositor
Resolution (Å)	48.85 – 2.05 48.85 – 2.05	Depositor EDS
% Data completeness (in resolution range)	96.6 (48.85-2.05) 96.7 (48.85-2.05)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.97 (at 2.05Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, R_{free}	0.180 , 0.212 0.182 , 0.212	Depositor DCC
R_{free} test set	3840 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	62.6	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 74.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	8899	wwPDB-VP
Average B, all atoms (Å^2)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.01% 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: DMS, MG, SO4, K5C, EDO

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	0.26	0/4706	0.44	0/6400
2	B	0.27	0/3564	0.44	0/4839
All	All	0.26	0/8270	0.44	0/11239

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	4586	0	4634	147	0
2	B	3465	0	3493	77	0
3	A	40	0	0	2	0
4	A	1	0	0	0	0
5	A	25	0	0	0	0
5	B	15	0	0	1	0
6	A	88	0	132	34	0
6	B	36	0	54	8	0
7	B	4	0	6	3	0
8	A	356	0	0	15	0
8	B	283	0	0	13	0
All	All	8899	0	8319	228	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 14.

All (228) 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:A:388:LYS:HG3	6:A:619:EDO:H21	1.25	1.08
1:A:551:LEU:HD21	6:A:620:EDO:H21	1.37	1.03
1:A:101:LYS:HE3	6:A:623:EDO:H11	1.39	1.01
1:A:65:LYS:HB2	1:A:68:SER:HB2	1.49	0.94
1:A:338[A]:THR:HG22	8:A:718:HOH:O	1.66	0.94
2:B:239:TRP:HB3	2:B:350:LYS:HE2	1.52	0.92
1:A:94:ILE:HG21	1:A:230:MET:HE2	1.60	0.83
1:A:63:ILE:HG22	1:A:64:LYS:H	1.46	0.81
1:A:136:ASN:H	6:A:627:EDO:C1	1.95	0.79
2:B:228:LEU:CD2	2:B:230:MET:HB3	2.13	0.78
1:A:353:LYS:H	6:A:612:EDO:H21	1.47	0.78
1:A:242:GLN:HB3	1:A:243:PRO:HD2	1.66	0.78
1:A:136:ASN:H	6:A:627:EDO:H11	1.48	0.78
2:B:91:GLN:HG3	2:B:92:LEU:H	1.50	0.77
1:A:543:GLY:HA3	2:B:283:LEU:O	1.85	0.77
1:A:85:GLN:HB2	6:A:624:EDO:H21	1.66	0.76
1:A:63:ILE:HB	1:A:72:ARG:HD3	1.67	0.76
2:B:107:THR:HA	2:B:232:TYR:O	1.85	0.75
1:A:359:GLY:HA3	8:A:904:HOH:O	1.85	0.75
1:A:478:GLU:HG2	8:A:850:HOH:O	1.86	0.74
6:A:612:EDO:H22	8:A:835:HOH:O	1.90	0.72
2:B:104:LYS:HA	2:B:237:ASP:OD1	1.88	0.72
2:B:354:TYR:CB	2:B:357:MET:HE2	2.21	0.71
2:B:353:LYS:H	6:B:508:EDO:H12	1.55	0.71
1:A:332:GLN:NE2	1:A:338[A]:THR:HG23	2.06	0.71
1:A:281:LYS:HE3	1:A:284:ARG:NH2	2.07	0.70
1:A:326[B]:ILE:HD13	1:A:388:LYS:HB2	1.74	0.69
2:B:354:TYR:HB3	2:B:357:MET:HE2	1.74	0.69
1:A:20[B]:LYS:HZ1	1:A:55:PRO:HB2	1.58	0.68
1:A:253:THR:HG22	1:A:292:VAL:HG12	1.76	0.68
1:A:297:GLU:O	1:A:301:LEU:HD13	1.95	0.67
1:A:114:ALA:HB1	1:A:214:LEU:HD13	1.77	0.66
2:B:195:ILE:O	2:B:199:ARG:HG3	1.94	0.66
2:B:108:VAL:HB	2:B:232:TYR:HB3	1.78	0.66
1:A:246:LEU:HD12	1:A:307:ARG:HG2	1.77	0.66
1:A:20[B]:LYS:NZ	1:A:55:PRO:HB2	2.11	0.66
1:A:259:LYS:NZ	1:A:263:LYS:HE3	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:LEU:O	1:A:264:LEU:HG	1.95	0.65
1:A:28:GLU:HG3	1:A:135:ILE:HD12	1.76	0.65
1:A:90:VAL:HG22	1:A:90:VAL:O	1.97	0.64
1:A:85:GLN:CB	6:A:624:EDO:H21	2.29	0.62
1:A:551:LEU:HD21	6:A:620:EDO:C2	2.21	0.62
2:B:386:THR:OG1	6:B:507:EDO:H12	1.99	0.62
1:A:255:ASN:HB2	1:A:289:LEU:HB3	1.81	0.62
1:A:388:LYS:CG	6:A:619:EDO:H21	2.17	0.61
2:B:353:LYS:H	6:B:508:EDO:C1	2.14	0.61
1:A:237:ASP:O	1:A:238:LYS:HD3	2.01	0.61
1:A:246:LEU:HD22	1:A:260:LEU:HD11	1.83	0.61
2:B:91:GLN:HG3	2:B:92:LEU:N	2.16	0.61
1:A:157:PRO:HG2	6:A:626:EDO:H22	1.81	0.61
2:B:360:ALA:HB2	2:B:366:LYS:HD3	1.82	0.61
1:A:208:HIS:O	1:A:211:ARG:HG2	2.01	0.60
7:B:501:DMS:H11	8:B:758:HOH:O	2.00	0.60
1:A:101:LYS:HD3	1:A:321:PRO:HG3	1.83	0.60
1:A:219:LYS:HG3	1:A:220:LYS:N	2.17	0.60
1:A:254:VAL:HG23	1:A:291:GLU:O	2.01	0.60
1:A:432:GLU:HG2	6:A:629:EDO:H21	1.83	0.60
2:B:336:GLN:HA	2:B:354:TYR:O	2.02	0.59
1:A:126:LYS:HE3	1:A:127:TYR:CE1	2.37	0.59
2:B:193:LEU:HD11	2:B:198:HIS:HA	1.85	0.59
2:B:367:GLN:HE22	6:B:512:EDO:C2	2.16	0.59
2:B:239:TRP:CB	2:B:350:LYS:HE2	2.29	0.58
8:A:877:HOH:O	2:B:394:GLN:HG3	2.02	0.58
1:A:266:TRP:O	1:A:269:GLN:HG2	2.04	0.58
1:A:507:GLN:HG2	8:A:792:HOH:O	2.03	0.57
1:A:127:TYR:OH	6:A:625:EDO:H22	2.05	0.57
1:A:178:ILE:HD11	1:A:180:ILE:HD11	1.85	0.57
1:A:17:ASP:O	1:A:83:ARG:HD3	2.03	0.57
2:B:281:LYS:O	2:B:284:ARG:HG2	2.04	0.57
1:A:259:LYS:HZ2	1:A:263:LYS:HE3	1.70	0.56
2:B:228:LEU:HD23	2:B:230:MET:HB3	1.86	0.56
2:B:174:GLN:NE2	2:B:204:GLU:OE2	2.39	0.56
1:A:372:VAL:HG11	1:A:411[A]:ILE:HG23	1.88	0.56
1:A:94:ILE:HD13	1:A:230:MET:HE3	1.88	0.56
1:A:181:CYS:HB2	8:B:825:HOH:O	2.06	0.56
2:B:8:VAL:HG21	2:B:159:ILE:HG23	1.88	0.56
1:A:308:GLU:O	1:A:311:LYS:HG2	2.05	0.55
2:B:61:PHE:CZ	2:B:74:LEU:HD23	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:GLU:HB3	1:A:225:PRO:HD2	1.87	0.55
1:A:279:LEU:HG	1:A:302:GLU:OE1	2.07	0.55
2:B:195:ILE:HD11	2:B:199:ARG:HH11	1.71	0.54
1:A:353:LYS:N	6:A:612:EDO:H21	2.21	0.54
1:A:227:PHE:HB3	3:A:601:K5C:N08	2.22	0.54
1:A:88:TRP:CZ2	6:B:510:EDO:H21	2.42	0.54
2:B:94:ILE:O	2:B:94:ILE:HD12	2.08	0.53
1:A:281:LYS:HE3	1:A:284:ARG:HH21	1.73	0.53
1:A:528:LYS:NZ	6:A:614:EDO:H11	2.23	0.53
2:B:353:LYS:O	6:B:508:EDO:H12	2.08	0.53
2:B:255:ASN:ND2	8:B:608:HOH:O	2.41	0.53
1:A:136:ASN:N	6:A:627:EDO:H11	2.21	0.53
2:B:317:VAL:HG12	2:B:349:LEU:HD23	1.90	0.53
1:A:314[B]:VAL:HG22	1:A:315[B]:HIS:N	2.24	0.52
1:A:544:GLY:N	2:B:285:GLY:O	2.42	0.52
1:A:388:LYS:HE3	6:A:619:EDO:H11	1.91	0.52
2:B:174:GLN:HG3	2:B:175:ASN:OD1	2.08	0.52
2:B:66:LYS:O	2:B:67:ASP:HB2	2.08	0.52
1:A:307:ARG:HB2	8:A:784:HOH:O	2.09	0.52
1:A:19:PRO:HG3	1:A:80:LEU:HB2	1.92	0.52
2:B:175:ASN:ND2	2:B:201:LYS:HD2	2.25	0.51
1:A:94:ILE:HD13	1:A:230:MET:CE	2.40	0.51
1:A:126:LYS:HE3	1:A:127:TYR:CZ	2.45	0.51
2:B:207:GLN:HA	2:B:207:GLN:OE1	2.10	0.51
1:A:246:LEU:HD22	1:A:260:LEU:CD1	2.40	0.51
1:A:63:ILE:HB	1:A:72:ARG:CD	2.37	0.51
1:A:101:LYS:HE3	6:A:623:EDO:C1	2.26	0.51
1:A:281:LYS:O	1:A:284:ARG:HG3	2.11	0.51
1:A:108:VAL:HG22	1:A:188:TYR:CD2	2.46	0.51
2:B:8:VAL:HG11	2:B:89:GLU:OE2	2.11	0.51
2:B:194:GLU:O	2:B:197:GLN:N	2.44	0.51
2:B:227:PHE:O	2:B:228:LEU:HB3	2.11	0.51
1:A:157:PRO:CG	6:A:626:EDO:H22	2.41	0.50
1:A:405:TYR:CE2	1:A:407:GLN:HB2	2.47	0.50
2:B:60[B]:VAL:HG12	2:B:75:VAL:HG22	1.94	0.50
2:B:317:VAL:CG1	2:B:349:LEU:HD23	2.41	0.50
1:A:326[B]:ILE:CD1	1:A:388:LYS:HB2	2.42	0.49
2:B:296:THR:O	2:B:300:GLU:HG3	2.12	0.49
6:A:618:EDO:H12	2:B:400:THR:O	2.12	0.49
1:A:244:ILE:HG22	1:A:310:LEU:HD13	1.94	0.49
1:A:260:LEU:HD21	1:A:303:LEU:HD13	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ILE:C	1:A:72:ARG:HG2	2.33	0.49
2:B:350:LYS:HG3	2:B:351:THR:N	2.28	0.49
1:A:118:VAL:HG11	1:A:149:LEU:HD11	1.94	0.49
1:A:332:GLN:CD	1:A:338[A]:THR:HG23	2.33	0.49
1:A:63:ILE:HG22	1:A:64:LYS:N	2.22	0.48
1:A:269:GLN:HA	1:A:351:THR:O	2.14	0.48
6:A:621:EDO:H11	8:A:996:HOH:O	2.11	0.48
2:B:201:LYS:NZ	2:B:204:GLU:OE1	2.39	0.48
1:A:7:THR:HG21	1:A:121:ASP:HA	1.94	0.48
1:A:273:GLY:HA2	1:A:338[A]:THR:HG21	1.95	0.48
1:A:290:THR:O	1:A:290:THR:HG22	2.14	0.48
1:A:135:ILE:HA	6:A:627:EDO:O1	2.14	0.47
1:A:480:GLN:NE2	8:A:722:HOH:O	2.46	0.47
2:B:70:LYS:HE2	8:B:850:HOH:O	2.14	0.47
1:A:23:GLN:HG2	1:A:133:PRO:HD3	1.96	0.47
1:A:28:GLU:O	1:A:32:LYS:HG2	2.14	0.47
1:A:432:GLU:CG	6:A:629:EDO:H21	2.43	0.47
2:B:362:THR:HG21	8:B:753:HOH:O	2.14	0.47
2:B:58:THR:HG23	2:B:76:ASP:O	2.15	0.47
1:A:63:ILE:HB	1:A:72:ARG:CG	2.43	0.47
1:A:240:THR:HB	1:A:315[A]:HIS:ND1	2.29	0.47
1:A:311:LYS:HG3	1:A:312:GLU:N	2.30	0.47
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.15	0.47
1:A:28:GLU:HG3	1:A:135:ILE:CD1	2.44	0.47
1:A:88:TRP:CH2	6:B:510:EDO:H21	2.50	0.47
2:B:319:TYR:OH	2:B:385:LYS:HE2	2.15	0.47
2:B:304:ALA:O	2:B:308:GLU:HG2	2.15	0.47
1:A:229:TRP:HB2	3:A:601:K5C:C07	2.46	0.46
2:B:191:SER:OG	2:B:198:HIS:ND1	2.36	0.46
1:A:134:SER:HA	8:A:861:HOH:O	2.14	0.46
2:B:240:THR:OG1	2:B:241:VAL:N	2.49	0.46
2:B:354:TYR:CD2	2:B:357:MET:HE1	2.51	0.46
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.98	0.45
1:A:178:ILE:CD1	1:A:180:ILE:HG13	2.46	0.45
2:B:229:TRP:CG	2:B:229:TRP:O	2.70	0.45
1:A:90:VAL:CG2	2:B:140:PRO:HB3	2.47	0.45
1:A:85:GLN:CA	6:A:624:EDO:H21	2.46	0.45
1:A:246:LEU:HG	1:A:310:LEU:HD12	1.98	0.45
2:B:357:MET:HB2	2:B:367:GLN:HG2	1.99	0.45
1:A:73:LYS:HE2	1:A:75:VAL:HG23	1.98	0.45
1:A:366:LYS:O	1:A:370:GLU:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:354:TYR:HB2	2:B:357:MET:HE2	1.98	0.45
2:B:423:VAL:HA	2:B:426:TRP:CD1	2.51	0.45
1:A:58:THR:HG23	1:A:76:ASP:O	2.17	0.45
1:A:136:ASN:O	1:A:138:GLU:HG3	2.16	0.45
1:A:379:SER:CB	1:A:387:PRO:HD3	2.46	0.45
2:B:312:GLU:HB3	2:B:313:PRO:HD2	1.97	0.45
2:B:228:LEU:HD22	8:B:611:HOH:O	2.17	0.44
1:A:474:ASN:HB2	6:A:611:EDO:H11	1.99	0.44
1:A:259:LYS:HZ1	1:A:263:LYS:HE3	1.81	0.44
1:A:314[B]:VAL:HG22	1:A:315[B]:HIS:H	1.82	0.44
1:A:398:TRP:CH2	1:A:411[A]:ILE:HG12	2.52	0.44
7:B:501:DMS:H12	8:B:607:HOH:O	2.17	0.44
1:A:339:TYR:CZ	1:A:352:GLY:HA3	2.52	0.44
1:A:547:GLN:O	1:A:550:LYS:HG2	2.18	0.44
1:A:89:GLU:O	1:A:92:LEU:HG	2.18	0.44
1:A:90:VAL:HG23	8:A:840:HOH:O	2.18	0.44
2:B:184:MET:HE3	8:B:768:HOH:O	2.17	0.44
1:A:88:TRP:HZ3	6:A:615:EDO:H11	1.82	0.43
2:B:228:LEU:HD23	2:B:230:MET:CB	2.47	0.43
1:A:182:GLN:HB3	1:A:187:LEU:CD1	2.48	0.43
1:A:380:ILE:CD1	7:B:501:DMS:H22	2.48	0.43
2:B:46:LYS:HD3	2:B:116:PHE:CD2	2.53	0.43
1:A:451:LYS:HB3	1:A:471:ASN:HA	2.00	0.43
2:B:88:TRP:HB3	2:B:91:GLN:O	2.18	0.43
2:B:189:VAL:HG21	2:B:205:LEU:CD2	2.48	0.43
1:A:65:LYS:HB2	1:A:68:SER:CB	2.34	0.43
2:B:8:VAL:O	2:B:10:VAL:HG23	2.18	0.43
1:A:166:LYS:HG2	6:A:609:EDO:H11	2.00	0.43
1:A:178:ILE:HD12	1:A:180:ILE:HG13	2.00	0.43
1:A:441:TYR:O	1:A:457:TYR:HA	2.19	0.43
2:B:183:TYR:CE2	2:B:184:MET:HG2	2.53	0.43
1:A:311:LYS:HG3	1:A:312:GLU:HG3	2.01	0.43
1:A:353:LYS:H	6:A:612:EDO:C2	2.24	0.43
2:B:162:SER:HB2	8:B:647:HOH:O	2.19	0.43
2:B:249[A]:LYS:NZ	8:B:621:HOH:O	2.52	0.42
1:A:85:GLN:HA	6:A:624:EDO:H21	2.01	0.42
1:A:134:SER:OG	1:A:137[A]:ASN:HA	2.19	0.42
2:B:13:LYS:HE3	2:B:84:THR:O	2.20	0.42
2:B:204:GLU:O	2:B:204:GLU:HG2	2.18	0.42
1:A:253:THR:HG22	1:A:292:VAL:CG1	2.46	0.42
6:A:618:EDO:H11	8:B:664:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:624:EDO:H22	5:B:502:SO4:O2	2.19	0.42
2:B:359:GLY:HA2	8:B:687:HOH:O	2.18	0.42
2:B:385:LYS:HB2	6:B:507:EDO:H21	2.01	0.42
1:A:108:VAL:HG22	1:A:188:TYR:CE2	2.54	0.42
2:B:210:LEU:O	2:B:210:LEU:HD23	2.19	0.42
1:A:419:THR:HG22	8:A:746:HOH:O	2.19	0.41
1:A:443:ASP:HB2	1:A:548:VAL:HG13	2.02	0.41
6:A:627:EDO:H12	8:A:872:HOH:O	2.19	0.41
1:A:353:LYS:HG2	6:A:612:EDO:H21	2.02	0.41
2:B:155:GLY:O	2:B:159:ILE:HG13	2.21	0.41
1:A:115:TYR:HA	1:A:160:PHE:CE1	2.56	0.41
1:A:122:GLU:HG3	8:A:923:HOH:O	2.20	0.41
1:A:129:ALA:HA	1:A:144:TYR:O	2.21	0.41
2:B:105:SER:O	2:B:190:GLY:HA2	2.21	0.41
1:A:253:THR:HA	1:A:292:VAL:HA	2.02	0.41
1:A:550:LYS:HD2	8:A:828:HOH:O	2.20	0.41
2:B:304:ALA:HA	8:B:755:HOH:O	2.21	0.41
1:A:458:VAL:HG12	1:A:464:GLN:HG2	2.03	0.40
1:A:183:TYR:CD2	1:A:229:TRP:HD1	2.40	0.40
1:A:210:LEU:HD23	1:A:210:LEU:HA	1.97	0.40
1:A:292:VAL:HG23	1:A:292:VAL:O	2.20	0.40
2:B:91:GLN:CG	2:B:92:LEU:H	2.26	0.40
1:A:101:LYS:HD3	1:A:321:PRO:CG	2.51	0.40
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.56	0.40
1:A:156:SER:HB2	1:A:157:PRO:HD3	2.03	0.40
1:A:39:THR:O	1:A:43:LYS:HG3	2.22	0.40
1:A:439:THR:O	1:A:459:THR:HA	2.22	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	563/557 (101%)	545 (97%)	17 (3%)	1 (0%)	47	39
2	B	415/428 (97%)	398 (96%)	16 (4%)	1 (0%)	47	39
All	All	978/985 (99%)	943 (96%)	33 (3%)	2 (0%)	47	39

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	356	ARG
1	A	90	VAL

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	504/495 (102%)	501 (99%)	3 (1%)	86	87
2	B	381/390 (98%)	376 (99%)	5 (1%)	69	67
All	All	885/885 (100%)	877 (99%)	8 (1%)	78	79

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	181	CYS
1	A	184	MET
1	A	192	ASP
2	B	227	PHE
2	B	232	TYR
2	B	233	GLU
2	B	358	ARG
2	B	394	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 42 ligands modelled in this entry, 1 is monoatomic - leaving 41 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	EDO	A	628	-	3,3,3	0.48	0	2,2,2	0.23	0
6	EDO	A	626	-	3,3,3	0.46	0	2,2,2	0.32	0
5	SO4	A	603	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	A	606	-	4,4,4	0.14	0	6,6,6	0.04	0
5	SO4	A	607	-	4,4,4	0.14	0	6,6,6	0.04	0
6	EDO	A	614	-	3,3,3	0.47	0	2,2,2	0.35	0
5	SO4	A	604	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	A	605	-	4,4,4	0.14	0	6,6,6	0.05	0
3	K5C	A	601	-	42,44,44	1.32	3 (7%)	51,63,63	2.15	16 (31%)
7	DMS	B	501	-	3,3,3	0.63	0	3,3,3	0.42	0
6	EDO	B	505	-	3,3,3	0.48	0	2,2,2	0.21	0
6	EDO	B	507	-	3,3,3	0.46	0	2,2,2	0.33	0
5	SO4	B	502	-	4,4,4	0.14	0	6,6,6	0.05	0
6	EDO	A	623	-	3,3,3	0.47	0	2,2,2	0.28	0
6	EDO	A	617	-	3,3,3	0.48	0	2,2,2	0.25	0
6	EDO	A	609	-	3,3,3	0.46	0	2,2,2	0.32	0
6	EDO	B	511	-	3,3,3	0.45	0	2,2,2	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	EDO	B	513	-	3,3,3	0.45	0	2,2,2	0.34	0
5	SO4	B	503	-	4,4,4	0.14	0	6,6,6	0.04	0
6	EDO	A	618	-	3,3,3	0.44	0	2,2,2	0.41	0
6	EDO	A	629	-	3,3,3	0.46	0	2,2,2	0.35	0
6	EDO	A	613	-	3,3,3	0.46	0	2,2,2	0.34	0
6	EDO	A	621	-	3,3,3	0.46	0	2,2,2	0.33	0
6	EDO	B	506	-	3,3,3	0.46	0	2,2,2	0.35	0
6	EDO	B	510	-	3,3,3	0.46	0	2,2,2	0.35	0
6	EDO	A	625	-	3,3,3	0.46	0	2,2,2	0.34	0
6	EDO	B	509	-	3,3,3	0.45	0	2,2,2	0.37	0
6	EDO	B	512	-	3,3,3	0.46	0	2,2,2	0.35	0
6	EDO	A	615	-	3,3,3	0.44	0	2,2,2	0.45	0
6	EDO	A	612	-	3,3,3	0.45	0	2,2,2	0.33	0
6	EDO	A	622	-	3,3,3	0.45	0	2,2,2	0.36	0
6	EDO	B	508	-	3,3,3	0.46	0	2,2,2	0.32	0
6	EDO	A	624	-	3,3,3	0.46	0	2,2,2	0.33	0
6	EDO	A	616	-	3,3,3	0.47	0	2,2,2	0.26	0
6	EDO	A	608	-	3,3,3	0.45	0	2,2,2	0.36	0
6	EDO	A	619	-	3,3,3	0.45	0	2,2,2	0.38	0
6	EDO	A	610	-	3,3,3	0.45	0	2,2,2	0.35	0
6	EDO	A	627	-	3,3,3	0.43	0	2,2,2	0.35	0
6	EDO	A	620	-	3,3,3	0.46	0	2,2,2	0.30	0
6	EDO	A	611	-	3,3,3	0.45	0	2,2,2	0.36	0
5	SO4	B	504	-	4,4,4	0.15	0	6,6,6	0.05	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
6	EDO	A	628	-	-	1/1/1/1	-
6	EDO	A	626	-	-	0/1/1/1	-
6	EDO	A	614	-	-	1/1/1/1	-
3	K5C	A	601	-	-	2/21/32/32	0/5/5/5
6	EDO	B	505	-	-	0/1/1/1	-
6	EDO	B	507	-	-	0/1/1/1	-
6	EDO	A	623	-	-	0/1/1/1	-
6	EDO	A	617	-	-	0/1/1/1	-
6	EDO	A	609	-	-	0/1/1/1	-
6	EDO	B	511	-	-	1/1/1/1	-
6	EDO	B	513	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	A	618	-	-	0/1/1/1	-
6	EDO	A	629	-	-	1/1/1/1	-
6	EDO	A	613	-	-	0/1/1/1	-
6	EDO	A	621	-	-	0/1/1/1	-
6	EDO	B	510	-	-	1/1/1/1	-
6	EDO	A	625	-	-	0/1/1/1	-
6	EDO	B	509	-	-	1/1/1/1	-
6	EDO	B	512	-	-	1/1/1/1	-
6	EDO	A	615	-	-	1/1/1/1	-
6	EDO	A	612	-	-	1/1/1/1	-
6	EDO	A	622	-	-	0/1/1/1	-
6	EDO	B	508	-	-	0/1/1/1	-
6	EDO	A	624	-	-	1/1/1/1	-
6	EDO	A	616	-	-	0/1/1/1	-
6	EDO	A	608	-	-	0/1/1/1	-
6	EDO	A	619	-	-	1/1/1/1	-
6	EDO	A	610	-	-	0/1/1/1	-
6	EDO	A	627	-	-	1/1/1/1	-
6	EDO	A	620	-	-	0/1/1/1	-
6	EDO	A	611	-	-	0/1/1/1	-
6	EDO	B	506	-	-	0/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	K5C	C20-N21	3.23	1.55	1.46
3	A	601	K5C	C16-N17	3.15	1.38	1.34
3	A	601	K5C	S27-N28	2.89	1.66	1.60

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	601	K5C	C31-C26-C25	-5.93	112.16	120.44
3	A	601	K5C	C32-C31-C26	5.82	125.47	119.45
3	A	601	K5C	C24-C25-C26	4.61	124.22	119.45
3	A	601	K5C	C22-N21-C20	-4.52	101.00	111.06
3	A	601	K5C	C16-N17-C18	4.21	131.43	124.31
3	A	601	K5C	O29-S27-C26	3.19	110.91	107.35
3	A	601	K5C	C31-C26-S27	3.13	124.27	119.73
3	A	601	K5C	O30-S27-O29	-2.97	113.88	118.76
3	A	601	K5C	C33-N21-C20	2.94	115.45	108.83
3	A	601	K5C	O13-C14-C40	2.77	120.19	115.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	601	K5C	C01-C02-C03	2.65	124.38	119.49
3	A	601	K5C	C25-C26-S27	2.64	123.56	119.73
3	A	601	K5C	C09-C04-C03	-2.52	115.70	119.12
3	A	601	K5C	O13-C12-C02	2.25	123.25	118.35
3	A	601	K5C	C22-C23-C32	2.20	124.91	120.77
3	A	601	K5C	C34-C18-N17	-2.17	107.21	110.60

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	K5C	C03-C04-C05-C06
3	A	601	K5C	C09-C04-C05-C06
6	A	612	EDO	O1-C1-C2-O2
6	A	629	EDO	O1-C1-C2-O2
6	B	509	EDO	O1-C1-C2-O2
6	A	614	EDO	O1-C1-C2-O2
6	B	512	EDO	O1-C1-C2-O2
6	A	628	EDO	O1-C1-C2-O2
6	B	510	EDO	O1-C1-C2-O2
6	B	511	EDO	O1-C1-C2-O2
6	A	624	EDO	O1-C1-C2-O2
6	A	627	EDO	O1-C1-C2-O2
6	A	615	EDO	O1-C1-C2-O2
6	A	619	EDO	O1-C1-C2-O2

There are no ring outliers.

22 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	626	EDO	2	0
6	A	614	EDO	1	0
3	A	601	K5C	2	0
7	B	501	DMS	3	0
6	B	507	EDO	2	0
5	B	502	SO4	1	0
6	A	623	EDO	2	0
6	A	609	EDO	1	0
6	A	618	EDO	2	0
6	A	629	EDO	2	0
6	A	621	EDO	1	0

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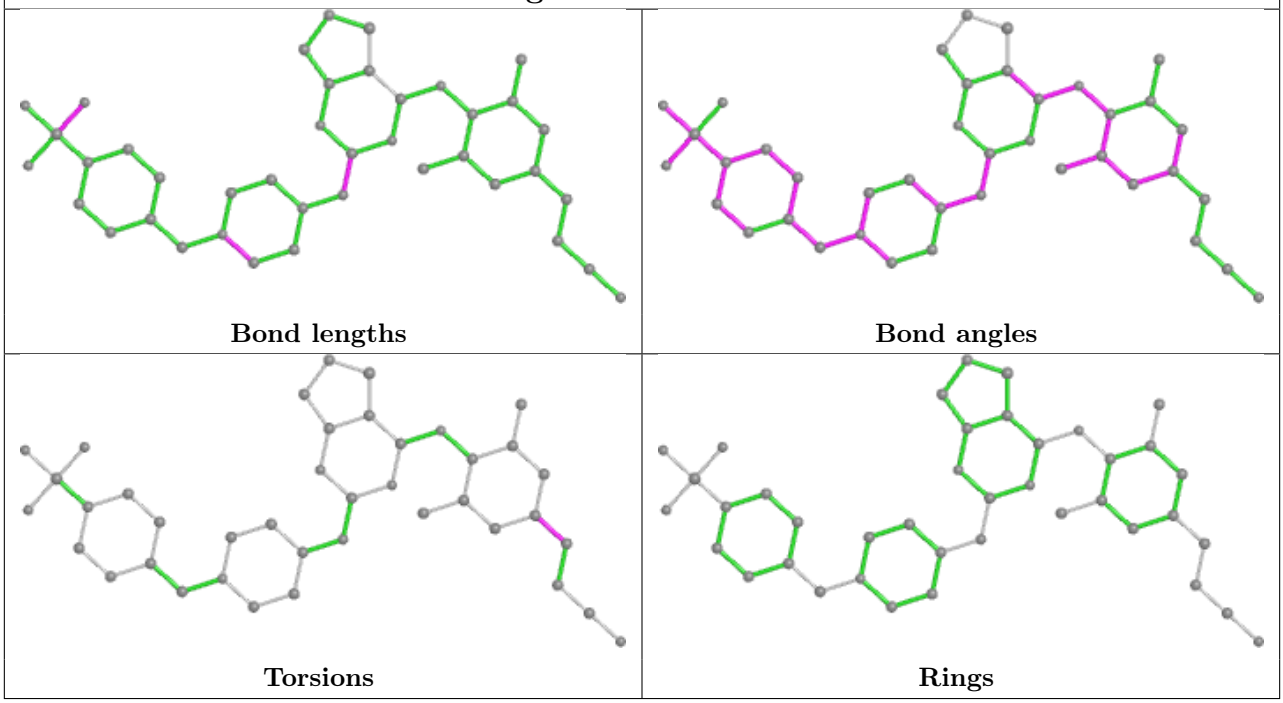
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	510	EDO	2	0
6	A	625	EDO	1	0
6	B	512	EDO	1	0
6	A	615	EDO	1	0
6	A	612	EDO	5	0
6	B	508	EDO	3	0
6	A	624	EDO	5	0
6	A	619	EDO	3	0
6	A	627	EDO	5	0
6	A	620	EDO	2	0
6	A	611	EDO	1	0

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 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 K5C A 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	556/557 (99%)	0.96	87 (15%)	2	1	47, 83, 179, 255	0
2	B	412/428 (96%)	0.90	56 (13%)	3	2	45, 75, 149, 259	0
All	All	968/985 (98%)	0.94	143 (14%)	2	1	45, 79, 171, 259	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	67	ASP	14.2
2	B	90	VAL	14.2
2	B	89	GLU	13.7
1	A	257	ILE	13.5
1	A	286	THR	12.8
1	A	290	THR	11.5
1	A	292	VAL	9.9
2	B	4	PRO	9.3
1	A	289	LEU	8.5
2	B	230	MET	8.2
1	A	68	SER	8.0
1	A	254	VAL	7.6
1	A	294	PRO	7.5
1	A	252	TRP	7.5
2	B	92	LEU	7.4
1	A	282	LEU	7.3
1	A	69	THR	7.2
1	A	293	ILE	7.1
1	A	288	ALA	6.9
1	A	301	LEU	6.7
1	A	283	LEU	6.7
1	A	260	LEU	6.6
2	B	232	TYR	6.3
2	B	210	LEU	6.1

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Mol	Chain	Res	Type	RSRZ
2	B	231	GLY	5.9
1	A	261	VAL	5.8
1	A	70	LYS	5.7
1	A	66	LYS	5.6
1	A	297	GLU	5.5
2	B	88	TRP	5.4
1	A	72	ARG	5.4
2	B	91	GLN	5.4
1	A	304	ALA	5.3
1	A	246	LEU	5.3
1	A	250	ASP	5.3
1	A	298	GLU	5.2
1	A	223	LYS	5.2
1	A	287	LYS	5.0
2	B	228	LEU	4.9
1	A	247	PRO	4.8
1	A	65	LYS	4.7
1	A	295	LEU	4.7
1	A	291	GLU	4.7
1	A	285	GLY	4.7
1	A	24	TRP	4.5
2	B	202	ILE	4.4
2	B	229	TRP	4.3
1	A	114	ALA	4.2
1	A	256	ASP	4.1
1	A	311	LYS	4.0
2	B	5	ILE	4.0
1	A	244	ILE	4.0
1	A	308	GLU	3.9
1	A	227	PHE	3.9
2	B	315	HIS	3.9
2	B	227	PHE	3.8
1	A	279	LEU	3.6
1	A	215	THR	3.6
1	A	284	ARG	3.6
1	A	255	ASN	3.6
2	B	212	TRP	3.5
1	A	116	PHE	3.4
1	A	108	VAL	3.4
2	B	87	PHE	3.4
2	B	197	GLN	3.4
2	B	67	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	302	GLU	3.3
1	A	251	SER	3.3
1	A	217	PRO	3.3
2	B	195	ILE	3.3
2	B	104	LYS	3.2
2	B	166	LYS	3.2
2	B	204	GLU	3.2
2	B	168	LEU	3.2
2	B	356	ARG	3.2
1	A	309	ILE	3.2
2	B	65	LYS	3.2
1	A	218	ASP	3.1
1	A	259	LYS	3.1
1	A	253	THR	3.1
1	A	275	LYS	3.1
1	A	221	HIS	3.0
1	A	248	GLU	3.0
1	A	312	GLU	3.0
1	A	111	VAL	2.9
2	B	357	MET	2.9
2	B	205	LEU	2.9
2	B	391	LEU	2.9
1	A	406	TRP	2.9
1	A	220	LYS	2.9
1	A	211	ARG	2.8
2	B	358	ARG	2.8
2	B	201	LYS	2.8
2	B	208	HIS	2.8
1	A	278	GLN	2.7
1	A	216	THR	2.6
2	B	7	THR	2.6
2	B	193	LEU	2.6
1	A	305	GLU	2.6
2	B	200	THR	2.6
1	A	315[A]	HIS	2.5
1	A	306	ASN	2.5
1	A	410[A]	TRP	2.5
1	A	271	TYR	2.4
2	B	393	ILE	2.4
1	A	264	LEU	2.4
2	B	325	LEU	2.4
1	A	398	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	237	ASP	2.4
1	A	91	GLN	2.4
2	B	203	GLU	2.3
1	A	360	ALA	2.3
1	A	299	ALA	2.3
2	B	354	TYR	2.3
1	A	93	GLY	2.3
2	B	14	PRO	2.3
2	B	207	GLN	2.3
1	A	61	PHE	2.2
2	B	206	ARG	2.2
1	A	64	LYS	2.2
1	A	546	GLU	2.2
2	B	169	GLU	2.2
1	A	281	LYS	2.2
2	B	173	LYS	2.2
2	B	198	HIS	2.2
2	B	209	LEU	2.2
2	B	318	TYR	2.2
2	B	338	THR	2.2
1	A	548	VAL	2.1
2	B	162	SER	2.1
2	B	233	GLU	2.1
1	A	109	LEU	2.1
2	B	365	VAL	2.1
1	A	92	LEU	2.1
2	B	368	LEU	2.1
2	B	69	THR	2.1
1	A	245	VAL	2.1
1	A	195	ILE	2.0
1	A	273	GLY	2.0
1	A	300	GLU	2.0
1	A	228	LEU	2.0
2	B	70	LYS	2.0
1	A	52	PRO	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	EDO	A	623	4/4	0.38	0.96	124,127,129,130	0
4	MG	A	602	1/1	0.44	0.51	105,105,105,105	0
6	EDO	B	512	4/4	0.44	0.47	111,111,115,118	0
6	EDO	A	628	4/4	0.47	0.21	98,102,105,109	0
6	EDO	A	625	4/4	0.47	0.39	114,114,116,117	0
6	EDO	B	508	4/4	0.55	0.39	96,96,97,104	0
6	EDO	A	620	4/4	0.60	0.47	143,143,143,143	4
6	EDO	A	610	4/4	0.68	0.23	79,85,93,98	0
6	EDO	A	629	4/4	0.68	0.43	107,108,108,111	0
6	EDO	A	626	4/4	0.74	0.19	106,107,108,109	0
6	EDO	A	609	4/4	0.78	0.29	115,116,119,121	0
6	EDO	A	614	4/4	0.78	0.17	68,73,77,84	0
6	EDO	B	507	4/4	0.79	0.21	88,91,95,98	0
6	EDO	A	616	4/4	0.80	0.22	98,99,100,101	0
6	EDO	A	611	4/4	0.80	0.15	83,87,88,95	0
6	EDO	B	510	4/4	0.81	0.37	106,106,107,108	0
6	EDO	A	622	4/4	0.81	0.19	95,97,100,105	0
6	EDO	B	509	4/4	0.82	0.24	97,98,99,104	0
6	EDO	A	617	4/4	0.82	0.29	74,84,85,88	0
6	EDO	A	624	4/4	0.82	0.20	102,104,105,105	0
6	EDO	A	619	4/4	0.83	0.33	79,80,86,87	0
6	EDO	A	621	4/4	0.83	0.34	77,89,101,104	0
6	EDO	B	513	4/4	0.84	0.23	108,112,115,119	0
5	SO4	A	605	5/5	0.85	0.13	120,126,130,132	0
6	EDO	A	618	4/4	0.85	0.35	104,104,104,107	0
6	EDO	A	627	4/4	0.86	0.28	94,96,100,104	0
6	EDO	A	615	4/4	0.86	0.18	89,90,90,93	0
6	EDO	A	608	4/4	0.86	0.20	91,93,97,99	0
5	SO4	B	502	5/5	0.89	0.24	139,142,143,149	0
6	EDO	A	612	4/4	0.89	0.15	108,108,110,113	0
6	EDO	B	511	4/4	0.90	0.48	80,89,95,100	0
5	SO4	B	503	5/5	0.90	0.29	150,151,152,153	0

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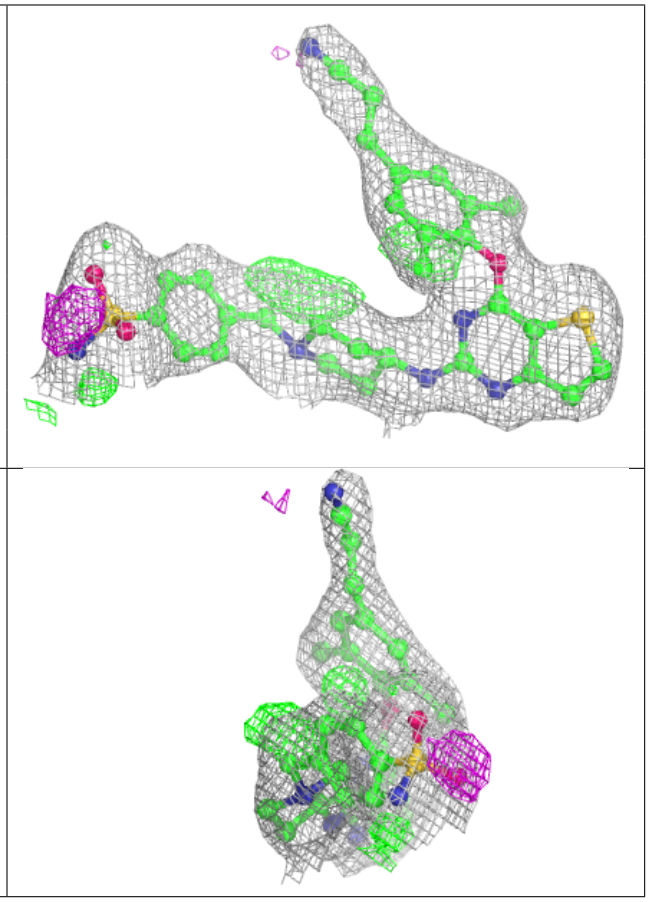
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	K5C	A	601	40/40	0.90	0.15	65,84,120,126	0
6	EDO	B	505	4/4	0.91	0.22	59,66,66,67	0
6	EDO	B	506	4/4	0.92	0.25	76,79,90,93	0
5	SO4	A	603	5/5	0.92	0.12	116,121,123,124	0
6	EDO	A	613	4/4	0.93	0.21	59,62,71,72	0
5	SO4	A	607	5/5	0.94	0.25	137,141,142,145	0
5	SO4	A	604	5/5	0.94	0.11	120,122,123,131	0
5	SO4	A	606	5/5	0.95	0.20	103,107,119,122	0
5	SO4	B	504	5/5	0.96	0.23	123,123,129,129	0
7	DMS	B	501	4/4	0.99	0.19	57,67,68,81	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 K5C 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.