Full wwPDB X-ray Structure Validation Report (i)

Apr 30, 2024 – 07:56 pm BST

PDB ID	:	4D2V
Title	:	Structure of MELK in complex with inhibitors
Authors	:	Johnson, C.N.; Berdini, V.; Beke, L.; Bonnet, P.; Brehmer, D.; Coyle, J.E.; Day, P.J.; Frederickson, M.; Freyne, E.J.E.; Gilissen, R.A.H.J.; Hamlett, C.C.F.; Howard, S.; Meerpoel, L.; McMenamin, R.; Patel, S.; Rees, D.C.; Sharff, A.; Sommen, F.; Wu, T.; Linders, J.T.M.
Deposited on	:	2014-05-13
Resolution	:	2.45 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:

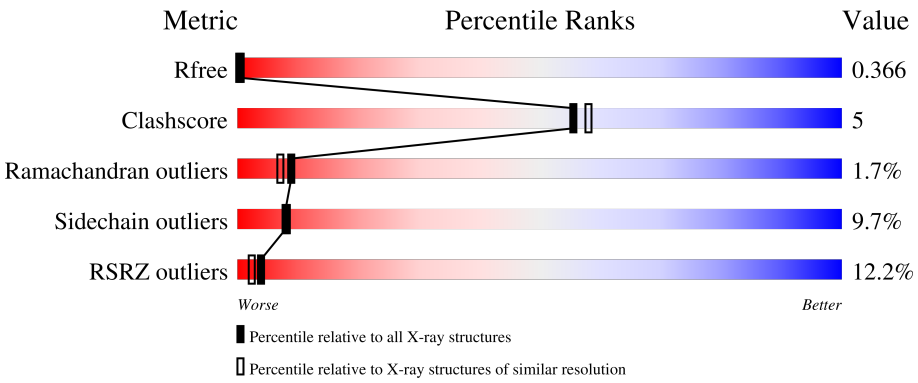
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	356	13% 72% 13% • 12%
1	B	356	12% 74% 14% • 10%
1	C	356	9% 74% 13% • 11%
1	D	356	10% 71% 16% • 11%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11042 atoms, of which 92 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 MATERNAL EMBRYONIC LEUCINE ZIPPER KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	313	2550	1645	429	459	17	0	1	0
1	B	322	2609	1679	442	471	17	0	1	0
1	C	316	2564	1655	431	461	17	0	0	0
1	D	318	2575	1662	436	461	16	0	0	0

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q14680
A	-18	GLY	-	expression tag	UNP Q14680
A	-17	SER	-	expression tag	UNP Q14680
A	-16	SER	-	expression tag	UNP Q14680
A	-15	HIS	-	expression tag	UNP Q14680
A	-14	HIS	-	expression tag	UNP Q14680
A	-13	HIS	-	expression tag	UNP Q14680
A	-12	HIS	-	expression tag	UNP Q14680
A	-11	HIS	-	expression tag	UNP Q14680
A	-10	HIS	-	expression tag	UNP Q14680
A	-9	SER	-	expression tag	UNP Q14680
A	-8	SER	-	expression tag	UNP Q14680
A	-7	GLY	-	expression tag	UNP Q14680
A	-6	LEU	-	expression tag	UNP Q14680
A	-5	VAL	-	expression tag	UNP Q14680
A	-4	PRO	-	expression tag	UNP Q14680
A	-3	ARG	-	expression tag	UNP Q14680
A	-2	GLY	-	expression tag	UNP Q14680
A	-1	SER	-	expression tag	UNP Q14680
A	0	HIS	-	expression tag	UNP Q14680
A	167	ALA	THR	engineered mutation	UNP Q14680

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Chain	Residue	Modelled	Actual	Comment	Reference
A	171	ALA	SER	engineered mutation	UNP Q14680
A	213	THR	ASN	engineered mutation	UNP Q14680
A	214	ALA	VAL	engineered mutation	UNP Q14680
A	215	ALA	MET	engineered mutation	UNP Q14680
A	218	VAL	TYR	engineered mutation	UNP Q14680
A	219	ALA	LYS	engineered mutation	UNP Q14680
B	-19	MET	-	expression tag	UNP Q14680
B	-18	GLY	-	expression tag	UNP Q14680
B	-17	SER	-	expression tag	UNP Q14680
B	-16	SER	-	expression tag	UNP Q14680
B	-15	HIS	-	expression tag	UNP Q14680
B	-14	HIS	-	expression tag	UNP Q14680
B	-13	HIS	-	expression tag	UNP Q14680
B	-12	HIS	-	expression tag	UNP Q14680
B	-11	HIS	-	expression tag	UNP Q14680
B	-10	HIS	-	expression tag	UNP Q14680
B	-9	SER	-	expression tag	UNP Q14680
B	-8	SER	-	expression tag	UNP Q14680
B	-7	GLY	-	expression tag	UNP Q14680
B	-6	LEU	-	expression tag	UNP Q14680
B	-5	VAL	-	expression tag	UNP Q14680
B	-4	PRO	-	expression tag	UNP Q14680
B	-3	ARG	-	expression tag	UNP Q14680
B	-2	GLY	-	expression tag	UNP Q14680
B	-1	SER	-	expression tag	UNP Q14680
B	0	HIS	-	expression tag	UNP Q14680
B	167	ALA	THR	engineered mutation	UNP Q14680
B	171	ALA	SER	engineered mutation	UNP Q14680
B	213	THR	ASN	engineered mutation	UNP Q14680
B	214	ALA	VAL	engineered mutation	UNP Q14680
B	215	ALA	MET	engineered mutation	UNP Q14680
B	218	VAL	TYR	engineered mutation	UNP Q14680
B	219	ALA	LYS	engineered mutation	UNP Q14680
C	-19	MET	-	expression tag	UNP Q14680
C	-18	GLY	-	expression tag	UNP Q14680
C	-17	SER	-	expression tag	UNP Q14680
C	-16	SER	-	expression tag	UNP Q14680
C	-15	HIS	-	expression tag	UNP Q14680
C	-14	HIS	-	expression tag	UNP Q14680
C	-13	HIS	-	expression tag	UNP Q14680
C	-12	HIS	-	expression tag	UNP Q14680
C	-11	HIS	-	expression tag	UNP Q14680

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	HIS	-	expression tag	UNP Q14680
C	-9	SER	-	expression tag	UNP Q14680
C	-8	SER	-	expression tag	UNP Q14680
C	-7	GLY	-	expression tag	UNP Q14680
C	-6	LEU	-	expression tag	UNP Q14680
C	-5	VAL	-	expression tag	UNP Q14680
C	-4	PRO	-	expression tag	UNP Q14680
C	-3	ARG	-	expression tag	UNP Q14680
C	-2	GLY	-	expression tag	UNP Q14680
C	-1	SER	-	expression tag	UNP Q14680
C	0	HIS	-	expression tag	UNP Q14680
C	167	ALA	THR	engineered mutation	UNP Q14680
C	171	ALA	SER	engineered mutation	UNP Q14680
C	213	THR	ASN	engineered mutation	UNP Q14680
C	214	ALA	VAL	engineered mutation	UNP Q14680
C	215	ALA	MET	engineered mutation	UNP Q14680
C	218	VAL	TYR	engineered mutation	UNP Q14680
C	219	ALA	LYS	engineered mutation	UNP Q14680
D	-19	MET	-	expression tag	UNP Q14680
D	-18	GLY	-	expression tag	UNP Q14680
D	-17	SER	-	expression tag	UNP Q14680
D	-16	SER	-	expression tag	UNP Q14680
D	-15	HIS	-	expression tag	UNP Q14680
D	-14	HIS	-	expression tag	UNP Q14680
D	-13	HIS	-	expression tag	UNP Q14680
D	-12	HIS	-	expression tag	UNP Q14680
D	-11	HIS	-	expression tag	UNP Q14680
D	-10	HIS	-	expression tag	UNP Q14680
D	-9	SER	-	expression tag	UNP Q14680
D	-8	SER	-	expression tag	UNP Q14680
D	-7	GLY	-	expression tag	UNP Q14680
D	-6	LEU	-	expression tag	UNP Q14680
D	-5	VAL	-	expression tag	UNP Q14680
D	-4	PRO	-	expression tag	UNP Q14680
D	-3	ARG	-	expression tag	UNP Q14680
D	-2	GLY	-	expression tag	UNP Q14680
D	-1	SER	-	expression tag	UNP Q14680
D	0	HIS	-	expression tag	UNP Q14680
D	167	ALA	THR	engineered mutation	UNP Q14680
D	171	ALA	SER	engineered mutation	UNP Q14680
D	213	THR	ASN	engineered mutation	UNP Q14680
D	214	ALA	VAL	engineered mutation	UNP Q14680

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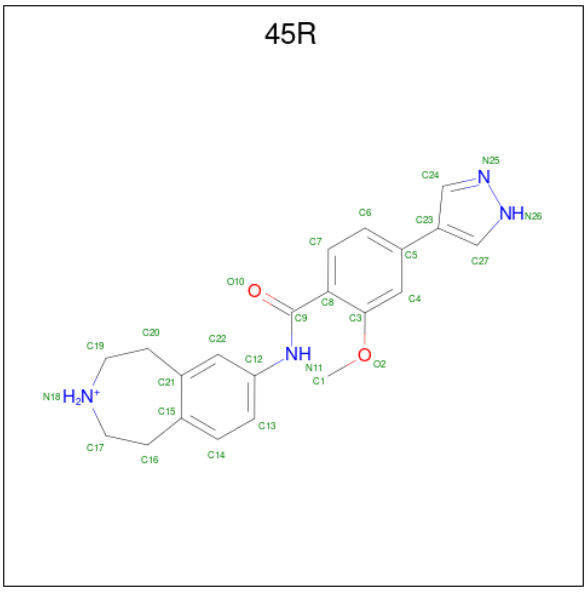
Chain	Residue	Modelled	Actual	Comment	Reference
D	215	ALA	MET	engineered mutation	UNP Q14680
D	218	VAL	TYR	engineered mutation	UNP Q14680
D	219	ALA	LYS	engineered mutation	UNP Q14680

- Molecule 2 is 7-{[2-methoxy-4-(1H-pyrazol-4-yl)benzoyl]amino}-2,3,4,5-tetrahydro-1H-3-benzazepinium (three-letter code: 45R) (formula: $C_{21}H_{23}N_4O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			50	21	23	4	2		
2	B	1	Total	C	H	N	O	0	0
			50	21	23	4	2		
2	C	1	Total	C	H	N	O	0	0
			50	21	23	4	2		
2	D	1	Total	C	H	N	O	0	0
			50	21	23	4	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	136	Total	O	0	0
			136	136		
3	B	147	Total	O	0	0
			147	147		
3	C	123	Total	O	0	0
			123	123		

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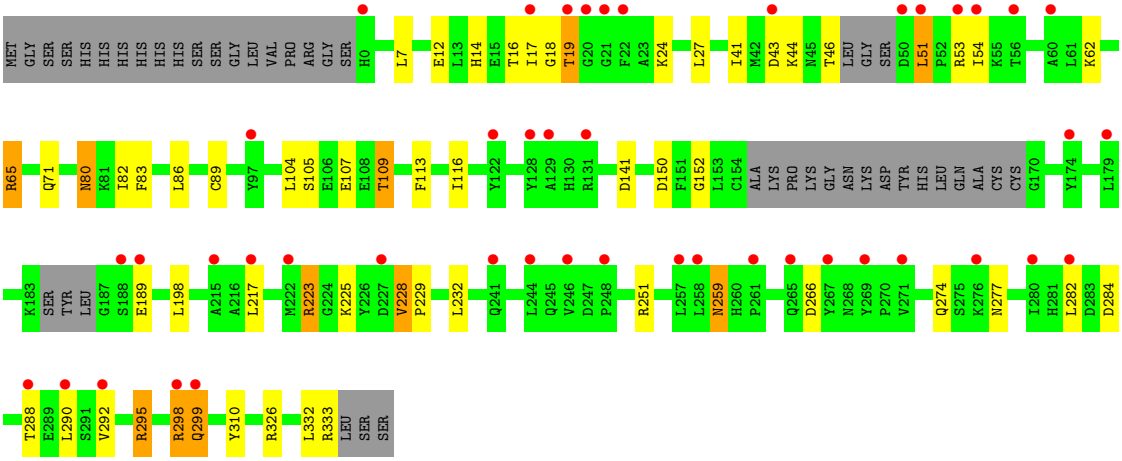
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	D	138	138	138	0	0

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.

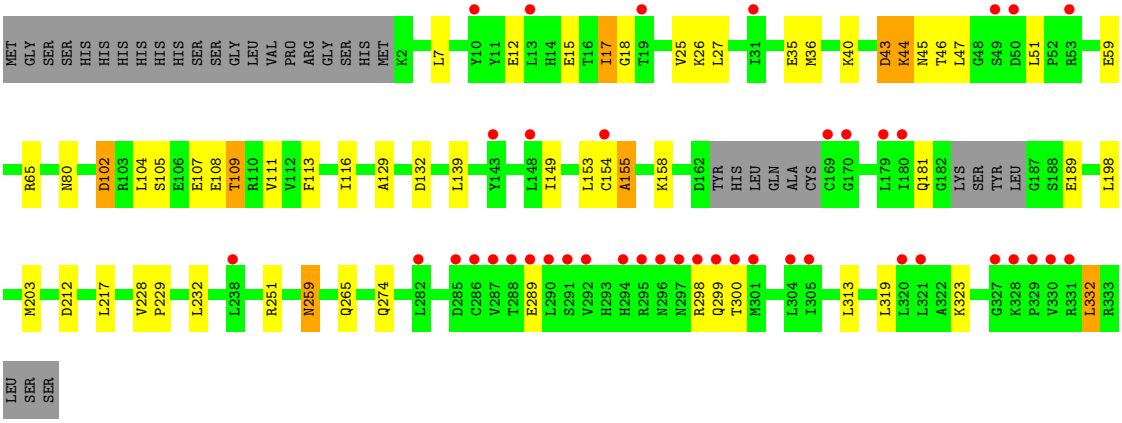
• Molecule 1: MATERNAL EMBRYONIC LEUCINE ZIPPER KINASE

Chain A:



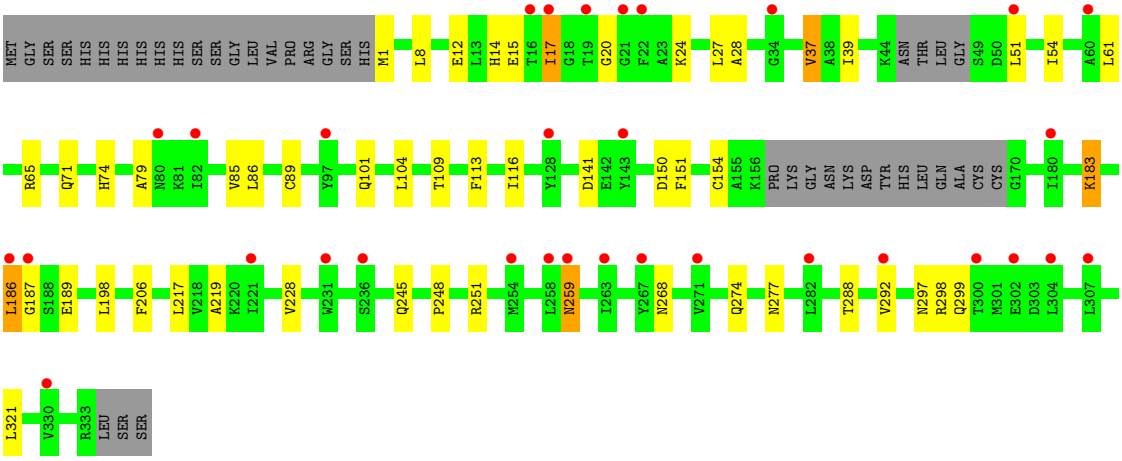
• Molecule 1: MATERNAL EMBRYONIC LEUCINE ZIPPER KINASE

Chain B:



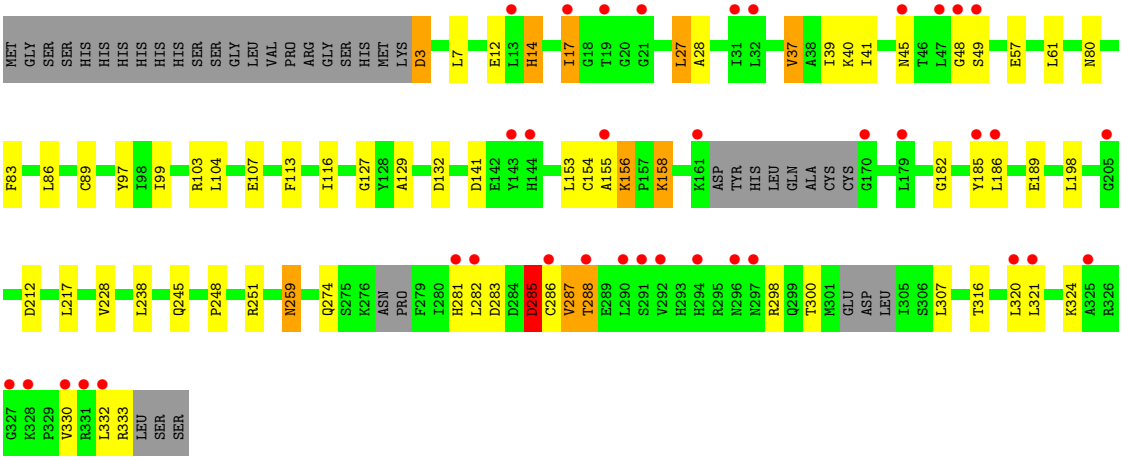
• Molecule 1: MATERNAL EMBRYONIC LEUCINE ZIPPER KINASE

Chain C:



- Molecule 1: MATERNAL EMBRYONIC LEUCINE ZIPPER KINASE

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	66.65Å 75.86Å 79.07Å 86.08° 69.45° 89.87°	Depositor
Resolution (Å)	48.69 – 2.45 47.60 – 2.45	Depositor EDS
% Data completeness (in resolution range)	94.6 (48.69-2.45) 94.6 (47.60-2.45)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.67 (at 2.45Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.291 , 0.357 0.287 , 0.366	Depositor DCC
R_{free} test set	2512 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	55.0	Xtriage
Anisotropy	0.368	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 95.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.54$, $< L^2 > = 0.38$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	11042	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.73% 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: 45R

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	0.55	0/2607	0.72	1/3525 (0.0%)
1	B	0.56	0/2670	0.71	0/3609
1	C	0.55	0/2622	0.71	0/3545
1	D	0.56	0/2632	0.74	0/3555
All	All	0.55	0/10531	0.72	1/14234 (0.0%)

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	B	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	18	GLY	C-N-CA	5.58	135.65	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	155	ALA	Peptide
1	D	285	ASP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2550	0	2556	23	0
1	B	2609	0	2629	30	0
1	C	2564	0	2582	24	0
1	D	2575	0	2602	31	0
2	A	27	23	23	2	0
2	B	27	23	23	3	0
2	C	27	23	23	2	0
2	D	27	23	23	4	0
3	A	136	0	0	2	0
3	B	147	0	0	3	0
3	C	123	0	0	0	0
3	D	138	0	0	3	0
All	All	10950	92	10461	106	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 5.

All (106) 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:C:248:PRO:HA	1:C:251:ARG:HG3	1.64	0.78
1:D:248:PRO:HA	1:D:251:ARG:HG3	1.67	0.77
1:B:43:ASP:HB3	1:B:46:THR:HB	1.70	0.73
1:D:129:ALA:H	1:D:155:ALA:CB	2.03	0.72
1:A:105:SER:O	1:A:109:THR:HG23	1.90	0.70
1:C:186:LEU:CB	1:C:187:GLY:HA2	2.23	0.68
1:D:129:ALA:H	1:D:155:ALA:HB3	1.59	0.68
1:D:3:ASP:HA	3:D:2003:HOH:O	1.94	0.68
1:B:17:ILE:CD1	1:B:27:LEU:HD13	2.26	0.66
1:A:17:ILE:HA	1:D:17:ILE:HD12	1.80	0.64
1:C:245:GLN:HB2	1:C:251:ARG:HG2	1.79	0.63
1:D:245:GLN:HB2	1:D:251:ARG:HG2	1.79	0.63
1:B:129:ALA:H	1:B:155:ALA:CB	2.11	0.62
1:B:139:LEU:CD2	1:B:149:ILE:HG12	2.29	0.62
1:C:186:LEU:HB3	1:C:187:GLY:HA2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:THR:HG22	1:A:298:ARG:HG3	1.81	0.62
2:B:1334:45R:H16	3:B:2034:HOH:O	2.00	0.61
1:B:129:ALA:H	1:B:155:ALA:HB3	1.65	0.61
1:D:17:ILE:HD11	2:D:1334:45R:H1A	1.83	0.60
1:D:17:ILE:O	1:D:17:ILE:HG13	2.02	0.59
1:C:183:LYS:HG2	1:C:186:LEU:HD13	1.85	0.59
1:B:108:GLU:HG2	3:B:2062:HOH:O	2.03	0.58
1:C:259:ASN:HD22	1:C:259:ASN:H	1.50	0.58
1:D:158:LYS:HE2	1:D:186:LEU:HD22	1.86	0.58
1:A:86:LEU:HD13	2:A:1334:45R:C27	2.33	0.58
1:B:18:GLY:HA3	1:B:25:VAL:H	1.69	0.58
1:B:104:LEU:HB2	1:B:109:THR:HG22	1.86	0.57
1:A:19:THR:HB	3:A:2012:HOH:O	2.03	0.57
1:A:44:LYS:HB3	1:A:82:ILE:HD11	1.87	0.56
1:D:57:GLU:HG3	1:D:61:LEU:HD23	1.86	0.56
1:D:259:ASN:HD22	1:D:259:ASN:H	1.53	0.56
1:B:212:ASP:O	1:C:79:ALA:HB2	2.06	0.55
1:B:17:ILE:HD11	1:B:27:LEU:HD13	1.89	0.55
1:C:186:LEU:CG	1:C:187:GLY:HA2	2.37	0.54
1:B:35:GLU:HB2	1:B:319:LEU:HD22	1.89	0.54
1:A:27:LEU:HD11	2:A:1334:45R:C13	2.38	0.53
1:A:65:ARG:HD2	1:A:71:GLN:HE22	1.73	0.53
1:B:105:SER:O	1:B:109:THR:HG23	2.08	0.53
1:D:288:THR:HG23	1:D:298:ARG:HE	1.75	0.52
1:B:139:LEU:HD21	1:B:149:ILE:CD1	2.40	0.52
1:A:259:ASN:HD22	1:A:259:ASN:H	1.57	0.52
1:C:104:LEU:HB2	1:C:109:THR:CG2	2.40	0.52
1:D:89:CYS:HA	1:D:141:ASP:HA	1.92	0.52
1:B:259:ASN:H	1:B:259:ASN:HD22	1.56	0.51
1:D:113:PHE:HA	1:D:116:ILE:HD12	1.92	0.51
1:C:113:PHE:HA	1:C:116:ILE:HD12	1.92	0.51
1:B:139:LEU:HD21	1:B:149:ILE:HG12	1.93	0.51
1:D:212:ASP:HB2	3:D:2097:HOH:O	2.10	0.51
1:C:51:LEU:HA	1:C:54:ILE:HG12	1.93	0.50
1:A:62:LYS:HG2	1:A:310:TYR:CD2	2.47	0.50
1:B:289:GLU:HG3	1:B:332:LEU:HD22	1.94	0.50
1:A:113:PHE:HA	1:A:116:ILE:HD12	1.93	0.49
1:D:132:ASP:HB2	1:D:153:LEU:HD12	1.94	0.49
1:A:228:VAL:HG21	3:A:2040:HOH:O	2.13	0.48
1:A:89:CYS:HA	1:A:141:ASP:HA	1.95	0.48
1:C:65:ARG:HG2	1:C:277:ASN:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:GLU:O	1:B:111:VAL:HG23	2.14	0.48
1:D:86:LEU:HD13	2:D:1334:45R:C14	2.45	0.47
1:B:17:ILE:HG21	2:B:1334:45R:H24	1.96	0.47
1:A:19:THR:HA	1:A:24:LYS:HB3	1.96	0.47
1:C:288:THR:O	1:C:292:VAL:HG13	2.14	0.47
1:B:109:THR:HG21	1:B:203:MET:CG	2.44	0.47
1:B:132:ASP:HB2	1:B:153:LEU:HD12	1.96	0.47
1:B:17:ILE:HG23	1:C:17:ILE:HG22	1.95	0.47
1:C:89:CYS:HA	1:C:141:ASP:HA	1.97	0.46
1:B:17:ILE:HD13	1:B:27:LEU:HD13	1.98	0.46
1:C:28:ALA:HB3	1:C:37:VAL:HG12	1.97	0.46
1:A:43:ASP:HA	1:A:80:ASN:O	2.15	0.46
1:D:14:HIS:HB2	1:D:27:LEU:HB3	1.97	0.46
1:B:229:PRO:HD2	1:B:232:LEU:HD22	1.98	0.45
1:B:139:LEU:HD22	1:B:139:LEU:N	2.30	0.45
1:C:186:LEU:HG	1:C:187:GLY:HA2	1.97	0.45
1:D:127:GLY:O	1:D:156:LYS:HA	2.17	0.45
1:D:286:CYS:O	1:D:287:VAL:HG23	2.16	0.45
2:D:1334:45R:H13	2:D:1334:45R:O10	2.15	0.45
1:B:36:MET:HB2	3:B:2016:HOH:O	2.16	0.44
1:C:186:LEU:HB3	1:C:187:GLY:CA	2.47	0.44
1:C:65:ARG:HG3	1:C:71:GLN:HE22	1.82	0.44
1:D:129:ALA:HB3	1:D:155:ALA:HB2	2.00	0.44
1:D:28:ALA:HB3	1:D:37:VAL:HG12	2.00	0.43
1:B:113:PHE:HA	1:B:116:ILE:HD12	2.00	0.43
1:D:97:TYR:CE2	1:D:104:LEU:HD11	2.53	0.43
1:A:284:ASP:O	1:A:288:THR:HG23	2.19	0.43
1:C:219:ALA:HB1	1:D:107:GLU:HB2	2.00	0.43
1:A:41:ILE:HG12	1:A:83:PHE:CD1	2.54	0.43
1:A:53:ARG:HD3	1:A:152:GLY:O	2.18	0.43
1:D:129:ALA:H	1:D:155:ALA:HB2	1.78	0.43
1:C:17:ILE:HD13	2:C:1334:45R:C22	2.49	0.43
1:C:86:LEU:HD13	2:C:1334:45R:C24	2.49	0.43
1:A:51:LEU:HA	1:A:54:ILE:HG12	2.00	0.42
1:A:223:ARG:HE	1:A:225:LYS:HB2	1.83	0.42
1:B:40:LYS:HE3	2:B:1334:45R:H19	2.00	0.42
1:D:285:ASP:HB3	1:D:330:VAL:HG11	2.02	0.42
1:B:129:ALA:HB3	1:B:155:ALA:HB2	2.02	0.42
1:D:316:THR:O	1:D:320:LEU:HB2	2.20	0.41
1:B:109:THR:HG21	1:B:203:MET:HG2	2.03	0.41
1:A:229:PRO:HD2	1:A:232:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:THR:O	1:A:292:VAL:HG13	2.19	0.41
1:D:7:LEU:HD11	1:D:39:ILE:HD13	2.02	0.41
1:C:61:LEU:HD11	1:C:151:PHE:CD1	2.55	0.41
1:C:74:HIS:HB3	1:C:85:VAL:CG2	2.50	0.41
1:B:109:THR:HG21	1:B:203:MET:HG3	2.03	0.41
1:D:40:LYS:HD2	2:D:1334:45R:H17	2.02	0.41
1:D:307:LEU:HB2	3:D:2132:HOH:O	2.19	0.41
1:D:41:ILE:HG12	1:D:83:PHE:CD1	2.56	0.40
1:A:65:ARG:HG2	1:A:277:ASN:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	306/356 (86%)	289 (94%)	12 (4%)	5 (2%)	9 8
1	B	317/356 (89%)	288 (91%)	26 (8%)	3 (1%)	17 19
1	C	310/356 (87%)	287 (93%)	17 (6%)	6 (2%)	8 6
1	D	310/356 (87%)	280 (90%)	23 (7%)	7 (2%)	6 4
All	All	1243/1424 (87%)	1144 (92%)	78 (6%)	21 (2%)	9 7

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	THR
1	A	298	ARG
1	C	17	ILE
1	D	287	VAL
1	B	15	GLU
1	D	48	GLY

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Mol	Chain	Res	Type
1	D	103	ARG
1	A	299	GLN
1	B	44	LYS
1	B	102	ASP
1	C	297	ASN
1	C	298	ARG
1	D	285	ASP
1	A	295	ARG
1	C	183	LYS
1	D	281	HIS
1	A	150	ASP
1	C	150	ASP
1	D	49	SER
1	C	20	GLY
1	D	182	GLY

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	277/314 (88%)	250 (90%)	27 (10%)	8 8
1	B	285/314 (91%)	254 (89%)	31 (11%)	6 6
1	C	279/314 (89%)	257 (92%)	22 (8%)	12 14
1	D	280/314 (89%)	252 (90%)	28 (10%)	7 7
All	All	1121/1256 (89%)	1013 (90%)	108 (10%)	8 8

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	12	GLU
1	A	14	HIS
1	A	16	THR
1	A	46	THR
1	A	51	LEU

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Mol	Chain	Res	Type
1	A	65	ARG
1	A	80	ASN
1	A	104	LEU
1	A	107	GLU
1	A	109	THR
1	A	189	GLU
1	A	198	LEU
1	A	217	LEU
1	A	223	ARG
1	A	228	VAL
1	A	251	ARG
1	A	259	ASN
1	A	266	ASP
1	A	274	GLN
1	A	282	LEU
1	A	290	LEU
1	A	295	ARG
1	A	299	GLN
1	A	326	ARG
1	A	332	LEU
1	A	333	ARG
1	B	7	LEU
1	B	12	GLU
1	B	17	ILE
1	B	26	LYS
1	B	43	ASP
1	B	44	LYS
1	B	45	ASN
1	B	47	LEU
1	B	51	LEU
1	B	59	GLU
1	B	65	ARG
1	B	80	ASN
1	B	102	ASP
1	B	109	THR
1	B	154	CYS
1	B	158	LYS
1	B	181	GLN
1	B	189	GLU
1	B	198	LEU
1	B	217	LEU
1	B	228	VAL

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Mol	Chain	Res	Type
1	B	251	ARG
1	B	259	ASN
1	B	265	GLN
1	B	274	GLN
1	B	298	ARG
1	B	299	GLN
1	B	300	THR
1	B	313	LEU
1	B	323	LYS
1	B	332	LEU
1	C	1	MET
1	C	8	LEU
1	C	12	GLU
1	C	14	HIS
1	C	15	GLU
1	C	24	LYS
1	C	27	LEU
1	C	37	VAL
1	C	39	ILE
1	C	101	GLN
1	C	154	CYS
1	C	186	LEU
1	C	189	GLU
1	C	198	LEU
1	C	206	PHE
1	C	217	LEU
1	C	228	VAL
1	C	259	ASN
1	C	268	ASN
1	C	274	GLN
1	C	299	GLN
1	C	321	LEU
1	D	3	ASP
1	D	12	GLU
1	D	14	HIS
1	D	17	ILE
1	D	27	LEU
1	D	37	VAL
1	D	45	ASN
1	D	80	ASN
1	D	99	ILE
1	D	154	CYS

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Mol	Chain	Res	Type
1	D	156	LYS
1	D	158	LYS
1	D	185	TYR
1	D	189	GLU
1	D	198	LEU
1	D	217	LEU
1	D	228	VAL
1	D	238	LEU
1	D	259	ASN
1	D	274	GLN
1	D	282	LEU
1	D	283	ASP
1	D	288	THR
1	D	300	THR
1	D	321	LEU
1	D	324	LYS
1	D	332	LEU
1	D	333	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	137	ASN
1	A	181	GLN
1	A	245	GLN
1	A	259	ASN
1	A	277	ASN
1	A	294	HIS
1	B	45	ASN
1	B	71	GLN
1	B	137	ASN
1	B	259	ASN
1	B	277	ASN
1	B	312	HIS
1	C	71	GLN
1	C	137	ASN
1	C	245	GLN
1	C	259	ASN
1	C	265	GLN
1	C	277	ASN
1	C	281	HIS

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Mol	Chain	Res	Type
1	C	312	HIS
1	D	71	GLN
1	D	137	ASN
1	D	245	GLN
1	D	259	ASN
1	D	265	GLN
1	D	312	HIS

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)

4 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	45R	B	1334	-	26,30,30	0.33	0	36,41,41	0.70	0
2	45R	C	1334	-	26,30,30	0.37	0	36,41,41	0.59	0
2	45R	A	1334	-	26,30,30	0.37	0	36,41,41	0.67	0
2	45R	D	1334	-	26,30,30	0.52	1 (3%)	36,41,41	0.93	2 (5%)

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	45R	B	1334	-	-	0/14/22/22	0/4/4/4
2	45R	C	1334	-	-	0/14/22/22	0/4/4/4
2	45R	A	1334	-	-	0/14/22/22	0/4/4/4
2	45R	D	1334	-	-	1/14/22/22	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1334	45R	O2-C3	2.04	1.40	1.37

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1334	45R	O2-C3-C8	2.16	119.70	116.55
2	D	1334	45R	O2-C3-C4	-2.12	120.47	124.12

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1334	45R	C4-C3-O2-C1

There are no ring outliers.

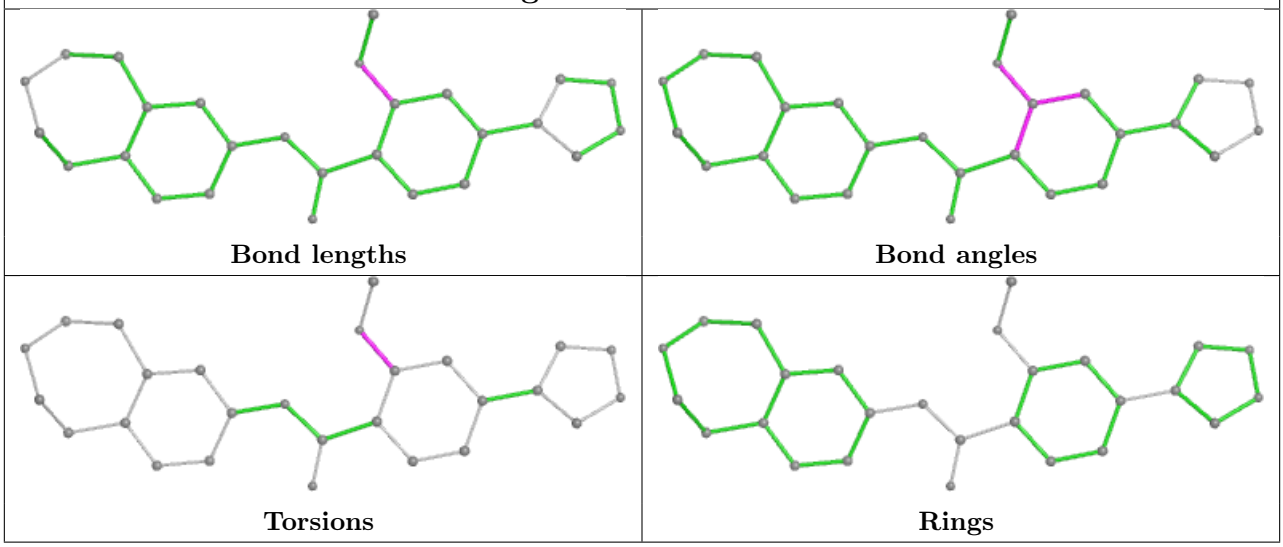
4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1334	45R	3	0
2	C	1334	45R	2	0
2	A	1334	45R	2	0
2	D	1334	45R	4	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 45R D 1334



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	313/356 (87%)	0.89	45 (14%)	2	1	40, 68, 101, 127	0
1	B	322/356 (90%)	1.01	41 (12%)	3	2	34, 67, 102, 123	0
1	C	316/356 (88%)	0.86	32 (10%)	7	4	42, 72, 105, 128	0
1	D	318/356 (89%)	0.78	37 (11%)	4	3	36, 65, 106, 131	0
All	All	1269/1424 (89%)	0.89	155 (12%)	4	2	34, 68, 105, 131	0

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	286	CYS	8.8
1	B	300	THR	6.6
1	A	179	LEU	6.4
1	C	186	LEU	6.2
1	B	327	GLY	6.2
1	D	186	LEU	5.9
1	A	271	VAL	5.8
1	C	292	VAL	5.3
1	C	304	LEU	5.3
1	C	80	ASN	5.1
1	B	330	VAL	5.1
1	D	327	GLY	5.0
1	B	292	VAL	4.8
1	B	180	ILE	4.8
1	D	331	ARG	4.6
1	A	22	PHE	4.6
1	B	297	ASN	4.5
1	B	287	VAL	4.4
1	A	288	THR	4.4
1	B	290	LEU	4.3
1	D	185	TYR	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	291	SER	3.9
1	C	22	PHE	3.9
1	A	248	PRO	3.8
1	B	294	HIS	3.7
1	B	179	LEU	3.7
1	D	144	HIS	3.7
1	B	288	THR	3.6
1	D	332	LEU	3.5
1	C	267	TYR	3.4
1	D	286	CYS	3.4
1	B	298	ARG	3.4
1	A	122	TYR	3.3
1	A	269	TYR	3.3
1	D	21	GLY	3.3
1	C	128	TYR	3.3
1	B	304	LEU	3.2
1	B	329	PRO	3.2
1	A	53	ARG	3.2
1	C	263	ILE	3.1
1	C	16	THR	3.1
1	B	49	SER	3.1
1	B	19	THR	3.1
1	A	292	VAL	3.1
1	D	143	TYR	3.1
1	D	291	SER	3.1
1	A	267	TYR	3.0
1	A	97[A]	TYR	3.0
1	A	215	ALA	3.0
1	B	299	GLN	3.0
1	A	217	LEU	3.0
1	D	292	VAL	3.0
1	B	320	LEU	3.0
1	D	45	ASN	3.0
1	C	236	SER	3.0
1	B	238	LEU	2.9
1	D	19	THR	2.9
1	D	320	LEU	2.9
1	D	328	LYS	2.9
1	A	50	ASP	2.9
1	D	290	LEU	2.9
1	A	222	MET	2.9
1	D	330	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	19	THR	2.9
1	D	179	LEU	2.9
1	C	271	VAL	2.8
1	C	51	LEU	2.8
1	D	205	GLY	2.8
1	B	305	ILE	2.8
1	B	169	CYS	2.8
1	C	307	LEU	2.8
1	A	265	GLN	2.8
1	A	188	SER	2.8
1	B	331	ARG	2.8
1	A	258	LEU	2.7
1	C	221	ILE	2.7
1	A	56	THR	2.7
1	C	17	ILE	2.7
1	A	276	LYS	2.6
1	D	296	ASN	2.6
1	B	321	LEU	2.6
1	C	254	MET	2.6
1	B	285	ASP	2.6
1	C	259	ASN	2.6
1	A	244	LEU	2.6
1	A	174	TYR	2.6
1	C	300	THR	2.6
1	D	32	LEU	2.5
1	D	294	HIS	2.5
1	B	328	LYS	2.5
1	C	143	TYR	2.5
1	B	295	ARG	2.5
1	B	31	ILE	2.5
1	A	299	GLN	2.5
1	D	49	SER	2.5
1	B	296	ASN	2.5
1	B	10	TYR	2.5
1	C	180	ILE	2.4
1	B	301	MET	2.4
1	A	189	GLU	2.4
1	A	128	TYR	2.4
1	D	17	ILE	2.4
1	A	129	ALA	2.4
1	B	282	LEU	2.4
1	D	13	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	330	VAL	2.4
1	C	82	ILE	2.4
1	D	297	ASN	2.4
1	A	43	ASP	2.4
1	C	258	LEU	2.4
1	C	231	TRP	2.4
1	D	155	ALA	2.4
1	C	34	GLY	2.3
1	A	227	ASP	2.3
1	D	31	ILE	2.3
1	A	51	LEU	2.3
1	D	161	LYS	2.3
1	B	50	ASP	2.3
1	B	148	LEU	2.3
1	A	17	ILE	2.3
1	D	321	LEU	2.3
1	D	282	LEU	2.3
1	B	13	LEU	2.2
1	D	325	ALA	2.2
1	A	19	THR	2.2
1	A	261	PRO	2.2
1	A	60	ALA	2.2
1	A	290	LEU	2.2
1	A	298	ARG	2.2
1	A	257	LEU	2.2
1	C	21	GLY	2.2
1	A	131	ARG	2.2
1	C	60	ALA	2.2
1	A	20	GLY	2.2
1	D	170	GLY	2.2
1	D	48	GLY	2.1
1	B	154	CYS	2.1
1	A	280	ILE	2.1
1	B	170	GLY	2.1
1	A	246	VAL	2.1
1	C	97	TYR	2.1
1	C	187	GLY	2.1
1	A	241	GLN	2.1
1	B	143	TYR	2.1
1	B	289	GLU	2.1
1	D	47	LEU	2.1
1	D	281	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	53	ARG	2.1
1	D	288	THR	2.1
1	A	282	LEU	2.1
1	A	21	GLY	2.1
1	C	302	GLU	2.1
1	A	0	HIS	2.1
1	A	54	ILE	2.0
1	C	282	LEU	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)

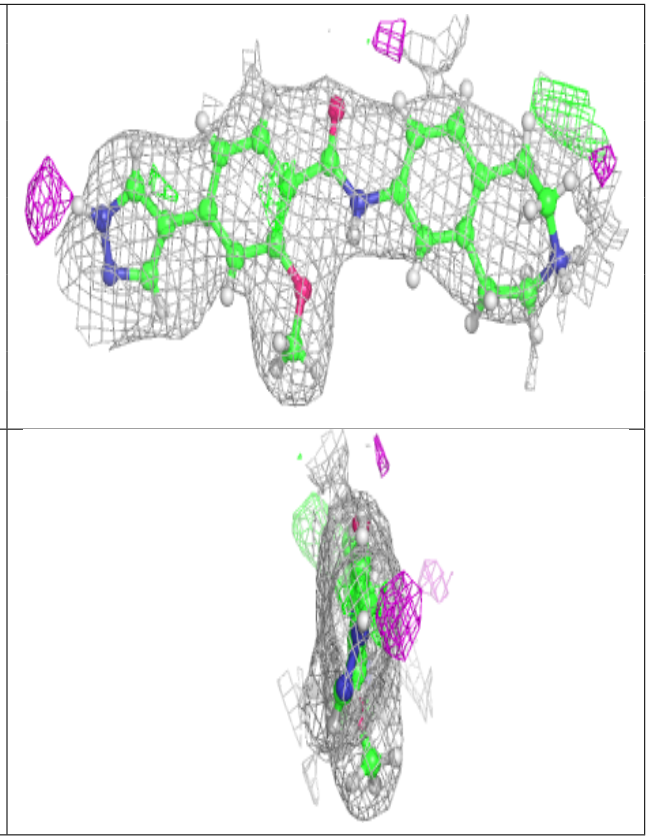
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	45R	B	1334	27/27	0.84	0.32	48,56,72,76	50
2	45R	D	1334	27/27	0.89	0.26	39,58,72,74	0
2	45R	A	1334	27/27	0.91	0.25	36,48,60,61	50
2	45R	C	1334	27/27	0.93	0.31	27,48,59,62	50

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 45R D 1334:

$2mF_o$-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.