

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	7P2T
Title	:	Tetartohedrally twinned crystal structure of Schistosoma mansoni HDAC8
		in complex with a tricyclic thieno[3,2-b]indole capped hydroxamate-based in-
		hibitor, bromine derivative
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Deposited on	:	2021-07-06
Resolution	:	2.30 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.30 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575(2.30-2.30)
Sidechain outliers	138945	5575(2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	А	440	9%	12% 9%
1	В	440	14%	13% • 8%
1	С	440	21%	17% • 7%
1	D	440	19%	15% 15%



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 12978 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Λ	402	Total	С	Ν	0	\mathbf{S}	0	0 2	0
	A	402	3230	2081	541	591	17	0	Δ	0
1	Р	406	Total	С	Ν	0	S	0	2	Ο
1	D	400	3262	2100	544	602	16	0	2	0
1	С	400	Total	С	Ν	0	S	0	1	0
	409	3286	2106	553	609	18	0	4		
1 D	374	Total	С	Ν	0	S	0	1	0	
	3/4	2991	1933	501	545	12	0		U	

• Molecule 1 is a protein called Histone deacetylase 8.

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	395	LYS	GLU	conflict	UNP A5H660
В	395	LYS	GLU	conflict	UNP A5H660
С	395	LYS	GLU	conflict	UNP A5H660
D	395	LYS	GLU	conflict	UNP A5H660

• Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total Zn 1 1	0	0
2	В	1	Total Zn 1 1	0	0
2	С	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

• Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	2	Total K 2 2	0	0
3	В	3	Total K 3 3	0	0
3	С	3	Total K 3 3	0	0
3	D	2	Total K 2 2	0	0

• Molecule 4 is 5-[[(2R)-7-bromanyl-2-phenyl-2,3-dihydrothieno[3,2-b]indol-4-yl]methyl]-N -oxidanyl-thiophene-2-carboxamide (three-letter code: 4VX) (formula: C₂₂H₁₇BrN₂O₂S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
	1	Total	Br	С	Ν	Ο	S	0	0	
4	Л	1	29	1	22	2	2	2	0	0
1	В	1	Total	Br	С	Ν	0	S	0	0
1	D	L	29	1	22	2	2	2	0	0
4	C	1	Total	Br	С	Ν	0	\mathbf{S}	0	0
4		1	29	1	22	2	2	2	0	0
	1	Total	Br	С	Ν	0	S	0	0	
4		I	29	1	22	2	2	2	0	0

• Molecule 5 is TRIS-HYDROXYMETHYL-METHYL-AMMONIUM (three-letter code: 144) (formula: $C_4H_{12}NO_3$).





Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{N} \\ 8 & 4 & 1 \end{array}$	O 3	0	0
5	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{N} \\ 8 & 4 & 1 \end{array}$	O 3	0	0

• Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total Cl 1 1	0	0

• Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	18	Total O 18 18	0	0
7	В	12	Total O 12 12	0	0
7	С	17	Total O 17 17	0	0
7	D	15	Total O 15 15	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: Histone deacetylase 8



• Molecule 1: Histone deacetylase 8





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	99.20Å 99.00Å 178.59Å	Depositor
a, b, c, α , β , γ	90.00° 91.30° 90.00°	Depositor
Besolution(A)	48.06 - 2.30	Depositor
Resolution (A)	47.70 - 2.30	EDS
% Data completeness	$100.0 \ (48.06-2.30)$	Depositor
(in resolution range)	93.6 (47.70-2.30)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.21	Depositor
$< I/\sigma(I) > 1$	$1.37 (at 2.29 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
D D	0.279 , 0.294	Depositor
κ, κ_{free}	0.276 , 0.298	DCC
R_{free} test set	3624 reflections $(4.72%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	46.0	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	(Not available), (Not available)	EDS
L-test for twinning ²	$< L >=0.37, < L^2>=0.19$	Xtriage
	0.269 for k,h,-l	
Estimated twinning fraction	0.276 for -k,-h,-l	Xtriage
	0.276 for -h,-k,l	
	0.480 for H, K, L	
Boported twinning fraction	0.189 for -K, -H, -L	Depositor
Reported twinning fraction	0.171 for K, H, -L	Depositor
	0.160 for h,-k,-l	
Outliers	0 of 76723 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	12978	wwPDB-VP
Average B, all atoms $(Å^2)$	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.93% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: 144, CL, K, 4VX, ZN

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

Mal	Chain	Bond lengths		Bond angles	
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.24	0/3326	0.45	0/4523
1	В	0.25	0/3358	0.45	0/4567
1	С	0.25	0/3388	0.47	0/4605
1	D	0.25	0/3075	0.46	0/4179
All	All	0.25	0/13147	0.46	0/17874

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	А	3230	0	3127	31	0
1	В	3262	0	3150	33	0
1	С	3286	0	3173	43	2
1	D	2991	0	2895	33	2
2	А	1	0	0	0	0
2	В	1	0	0	0	0
2	С	1	0	0	0	0
2	D	1	0	0	0	0
3	A	2	0	0	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	В	3	0	0	0	0
3	С	3	0	0	0	0
3	D	2	0	0	0	0
4	А	29	0	0	0	0
4	В	29	0	0	0	0
4	С	29	0	0	0	0
4	D	29	0	0	0	0
5	С	8	0	12	1	0
5	D	8	0	12	0	0
6	D	1	0	0	0	0
7	А	18	0	0	0	0
7	В	12	0	0	0	0
7	С	17	0	0	0	0
7	D	15	0	0	0	0
All	All	12978	0	12369	139	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (139)	close	$\operatorname{contacts}$	within	the same	e asymmetric	unit	are	listed	below,	sorted	by	their	clash
magnitud	e.												

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:129:HIS:HD1	1:C:130:CYS:HG	1.26	0.80
1:A:407:HIS:O	1:A:411:ILE:HG13	1.95	0.67
1:B:279:VAL:HG13	1:B:334:LEU:HD12	1.77	0.66
1:C:267:ASP:O	1:C:271:ILE:HG13	1.94	0.66
1:B:93:ASP:OD1	1:B:98:ASN:ND2	2.28	0.66
1:C:299:ASN:HB3	1:C:349:LEU:HD22	1.76	0.66
1:A:358:ILE:HG23	1:A:362:LYS:HD3	1.78	0.65
1:A:28:VAL:O	1:A:32:ILE:HG13	1.98	0.64
1:A:93:ASP:OD1	1:A:98:ASN:ND2	2.30	0.64
1:A:327:LEU:HD11	1:A:357:THR:HG22	1.80	0.63
1:C:221:THR:OG1	1:C:222:TRP:N	2.32	0.62
1:D:141:HIS:HD2	1:D:190:GLY:HA2	1.65	0.61
1:D:344:PRO:O	1:D:348:ARG:HG3	2.01	0.61
1:C:142:HIS:O	1:C:144:LYS:NZ	2.32	0.61
1:D:355:ALA:O	1:D:359:GLU:HG3	2.01	0.61
1:D:119:LEU:HD22	1:D:163:ARG:HE	1.66	0.60
1:B:292:HIS:HB3	1:B:294:ILE:HD13	1.85	0.58
1:C:112:LEU:O	1:C:116:GLN:HG3	2.02	0.58
1:C:272:VAL:HG23	1:C:273:ILE:HD12	1.86	0.57



	le de pagem	Interatomic	Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)		
1:A:354:THR:O	1:A:358:ILE:HG13	2.05	0.57		
1:D:266:LEU:HD11	1:D:325:LYS:HG3	1.85	0.57		
1:A:372:ILE:HG23	1:A:378:PHE:HE1	1.69	0.57		
1:C:278:VAL:HG13	1:C:333:THR:HG23	1.86	0.57		
1:D:182:TYR:HD1	1:D:279:VAL:HG13	1.69	0.56		
1:B:327:LEU:HD11	1:B:357:THR:HG22	1.87	0.56		
1:C:3:VAL:HB	1:C:41:LEU:HD12	1.87	0.56		
1:C:41:LEU:HD21	1:C:358:ILE:HD11	1.87	0.55		
1:C:24:ARG:HH21	1:C:350:TRP:HH2	1.54	0.55		
1:A:32:ILE:HG12	1:A:351:THR:HG22	1.88	0.55		
1:D:24:ARG:NH2	1:D:338:GLY:O	2.38	0.54		
1:B:287:LEU:HD11	1:B:349:LEU:HD22	1.90	0.53		
1:C:348:ARG:NH1	1:C:386:GLU:O	2.41	0.53		
1:B:126:ILE:HD11	1:B:164:LEU:HA	1.91	0.53		
1:A:157:ILE:O	1:A:161:ILE:HG13	2.09	0.53		
1:B:62:PHE:O	1:B:145:ARG:NH1	2.42	0.53		
1:A:402:ASP:HB3	1:A:405:GLN:HG2	1.91	0.52		
1:C:198:TRP:CH2	1:C:234:LEU:HD12	2.45	0.52		
1:D:135:ASN:HD22	1:D:336:LEU:HD11	1.74	0.52		
1:A:141:HIS:ND1	1:A:184:ASP:OD2	2.39	0.51		
1:C:129:HIS:ND1	1:C:130:CYS:SG	2.66	0.51		
1:B:32:ILE:HD13	1:B:351:THR:HG22	1.93	0.50		
1:B:104:PHE:H	1:B:107:VAL:HG23	1.77	0.50		
1:D:235:ASN:HA	1:D:244:ALA:HB3	1.94	0.50		
1:C:178:THR:HA	1:C:276:SER:HB2	1.94	0.50		
1:C:303:ASN:HD22	1:C:303:ASN:N	2.10	0.50		
1:C:78:HIS:CE1	1:C:82:LYS:HE3	2.47	0.50		
1:D:33:ASN:HA	1:D:38:ILE:HG12	1.92	0.50		
1:C:189:HIS:ND1	1:C:219:THR:HG23	2.27	0.49		
1:B:258:TRP:O	1:B:262:ILE:HG12	2.13	0.49		
1:C:307:ASP:OD1	1:C:307:ASP:N	2.43	0.49		
1:C:279:VAL:HG23	1:C:334:LEU:HD12	1.95	0.49		
1:C:254:ASN:HB2	1:C:394:HIS:CD2	2.47	0.48		
1:C:98:ASN:N	1:C:98:ASN:OD1	2.43	0.48		
1:D:38:ILE:HG13	1:D:39:PRO:HD3	1.96	0.48		
1:A:372:ILE:HD11	1:A:375:HIS:CE1	2.48	0.48		
1:B:139:GLY:N	1:B:336:LEU:HD22	2.29	0.48		
1:A:1:MET:N	1:A:361:VAL:HG12	2.29	0.48		
1:B:219:THR:OG1	1:B:220:GLY:N	2.45	0.48		
1:A:320:LEU:HD11	1:A:352:ARG:HE	1.78	0.47		
1:D:28:VAL:HG22	1:D:347:ALA:HA	1.96	0.47		



	Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)
1.D.182.TYR.HD2	1.D.205.THR.HG23	1.78	0.47
1:D:262:ILE:HG12	1:D:266:LEU:HD23	1.96	0.47
1.B.88.ASP.0	1.B:92.MET.HG2	2.15	0.47
1:A:372:ILE:HD11	1:A:375:HIS:HE1	1.80	0.47
1:D:182:TYR:HA	1:D:279:VAL:HG13	1.96	0.46
1:A:204:VAL:HG21	1:A·273·ILE·HG12	1.97	0.46
1.C.212.SEB.OG	1.C·215·PHE·HB2	2.16	0.46
1:D:354:THR:O	1:D:357:THR:OG1	2.29	0.45
1:C:303:ASN:OD1	5:C:505:144:O2	2.32	0.45
1:D:374:GLU:HA	1:D:378:PHE:CD1	2.52	0.45
1:A:112:LEU:O	1:A·116·GLN·HG3	2.16	0.45
1:A:182:TYR:HA	1:A:279:VAL:HG13	1.97	0.45
1:A:118:SER:OG	1:A:156:ASP:OD2	2.33	0.45
1:D:139:GLY:N	1:D:336:LEU:HD12	2.31	0.45
1.C.208.VAL:HG21	1:C:262:ILE:HD11	1 99	0.45
1.D.6.VAL:HA	1.D.44.VAL:O	2.16	0.45
1.D.288.ALA.HB2	1.D.296.ABG.HA	1.98	0.45
1:D:355:ALA:HA	1:D:358:ILE:HD12	1.99	0.45
1:A:344:PRO:0	1:A:348:ARG:HG3	2.18	0.44
1:B:189:HIS:CD2	1:B:219:THB:HG23	2.52	0.44
1:C:299:ASN:HB3	1:C:349:LEU:CD2	2.45	0.44
1:A:219:THR:OG1	1:A:220:GLY:N	2.50	0.44
1:C:75:GLN:OE1	1:C:108:PHE:HB3	2.17	0.44
1:B:266:LEU:HB2	1:B:325:LYS:NZ	2.32	0.44
1:A:278:VAL:O	1:A:333:THR:HA	2.18	0.44
1:A:419:ALA:HA	1:A:424:LEU:HD12	1.98	0.44
1:C:266:LEU:HD12	1:C:329:TRP:HH2	1.83	0.44
1:B:141:HIS:HD2	1:B:190:GLY:HA2	1.83	0.44
1:C:104:PHE:O	1:C:107:VAL:HG23	2.17	0.44
1:C:80:GLU:OE1	1:C:81:GLU:N	2.51	0.44
1:C:99:TYR:HB2	1:C:100:ASP:H	1.65	0.43
1:B:118:SER:OG	1:B:156:ASP:OD2	2.35	0.43
1:D:24:ARG:HD3	1:D:343:PHE:CD1	2.53	0.43
1:D:206:PHE:HA	1:D:245:PHE:O	2.17	0.43
1:B:57:GLU:HA	1:B:60:THR:HG22	2.00	0.43
1:C:52:PRO:O	1:C:55:MET:HG3	2.18	0.43
1:D:135:ASN:HD22	1:D:336:LEU:CD1	2.32	0.43
1:B:430:GLN:OE1	1:B:433:GLN:NE2	2.41	0.43
1:C:30:ASP:OD1	1:C:31:LEU:N	2.52	0.43
1:D:161:ILE:O	1:D:165:VAL:HG22	2.19	0.43
1:C:268:SER:O	1:C:272:VAL:HG22	2.18	0.43



	Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:75:GLN:OE1	1:D:108:PHE:N	2.51	0.42
1:A:182:TYR:HD2	1:A:205:THR:HG23	1.85	0.42
1:D:29:MET:HA	1:D:32:ILE:HD12	2.02	0.42
1:D:350:TRP:HA	1:D:353:VAL:HG22	2.02	0.42
1:A:182:TYR:HD1	1:A:279:VAL:HG13	1.85	0.42
1:B:3:VAL:HG13	1:B:361:VAL:HG11	2.01	0.42
1:B:175:ASN:OD1	1:B:175:ASN:N	2.53	0.42
1:C:182:TYR:HD1	1:C:279:VAL:HG13	1.83	0.42
1:C:183:VAL:HG13	1:C:280:VAL:HG13	2.02	0.42
1:C:201:PRO:HG3	1:C:239:ARG:HB3	2.00	0.42
1:D:348:ARG:HE	1:D:372:ILE:HD11	1.85	0.42
1:A:75:GLN:NE2	1:A:109:ASP:OD2	2.53	0.41
1:B:421:LEU:HD13	1:C:306:LEU:H	1.84	0.41
1:C:104:PHE:H	1:C:107:VAL:HG23	1.85	0.41
1:A:345:ASP:HA	1:A:348:ARG:HD2	2.03	0.41
1:B:70:ALA:O	1:B:73:LYS:HG3	2.20	0.41
1:C:245:PHE:HD2	1:C:411:ILE:HG23	1.85	0.41
1:C:104:PHE:CE1	1:C:107:VAL:HG22	2.55	0.41
1:B:4:GLY:O	1:B:134:ILE:N	2.45	0.41
1:A:28:VAL:HG22	1:A:347:ALA:HA	2.02	0.41
1:B:266:LEU:HB2	1:B:325:LYS:HZ1	1.86	0.41
1:D:259:SER:HA	1:D:262:ILE:HG22	2.02	0.41
1:A:1:MET:H3	1:A:361:VAL:HG12	1.86	0.41
1:A:288:ALA:HB2	1:A:296:ARG:HA	2.02	0.41
1:B:404:ILE:HG12	1:B:405:GLN:N	2.36	0.41
1:D:287:LEU:HD21	1:D:349:LEU:HD22	2.03	0.41
1:C:3:VAL:HG13	1:C:361:VAL:HG11	2.03	0.41
1:B:285:ASP:OD1	1:B:285:ASP:N	2.49	0.41
1:C:288:ALA:HB2	1:C:296:ARG:HA	2.03	0.41
1:B:75:GLN:OE1	1:B:108:PHE:N	2.54	0.40
1:B:98:ASN:N	1:B:98:ASN:OD1	2.54	0.40
1:D:56:TYR:OH	1:D:65:THR:HG23	2.20	0.40
1:B:372:ILE:O	1:B:372:ILE:HG13	2.21	0.40
1:A:164:LEU:HD12	1:A:277:TYR:CD1	2.56	0.40
1:B:104:PHE:H	1:B:107:VAL:CG2	2.35	0.40
1:D:419:ALA:O	1:D:423:LYS:N	2.54	0.40
1:B:112:LEU:O	1:B:116:GLN:HG3	2.22	0.40
1:B:132:VAL:HA	1:B:333:THR:O	2.22	0.40

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



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:PRO:O	1:D:90:LEU:CD2[3_555]	1.97	0.23
1:C:83:GLU:CB	1:D:371:GLU:O[2_556]	2.12	0.08

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	Perce	ntiles
1	А	392/440~(89%)	379~(97%)	13 (3%)	0	100	100
1	В	398/440~(90%)	387~(97%)	11 (3%)	0	100	100
1	С	405/440~(92%)	383~(95%)	21 (5%)	1 (0%)	47	58
1	D	357/440~(81%)	349~(98%)	8 (2%)	0	100	100
All	All	1552/1760~(88%)	1498 (96%)	53 (3%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	С	277	TYR

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	А	352/386~(91%)	345~(98%)	7~(2%)	55 72		
1	В	355/386~(92%)	343~(97%)	12 (3%)	37 51		
1	С	360/386~(93%)	344~(96%)	16 (4%)	28 39		



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	D	323/386~(84%)	310 (96%)	13 (4%)	31 44		
All	All	1390/1544~(90%)	1342~(96%)	48 (4%)	36 50		

All (48) residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	А	141	HIS
1	А	176	ARG
1	А	217	PRO
1	А	301	TYR
1	А	334	LEU
1	А	342	ASN
1	А	365	LYS
1	В	3	VAL
1	В	41	LEU
1	В	73	LYS
1	В	91	LEU
1	В	128	ARG
1	В	154	LEU
1	В	162	HIS
1	В	247	LEU
1	В	301	TYR
1	В	404	ILE
1	В	405	GLN
1	В	425	ILE
1	С	3	VAL
1	С	5	ILE
1	С	24	ARG
1	С	30	ASP
1	С	99	TYR
1	С	109	ASP
1	С	141	HIS
1	С	234	LEU
1	С	247	LEU
1	С	301	TYR
1	С	303	ASN
1	С	309	ASP
1	С	342	ASN
1	С	352	ARG
1	С	404	ILE
1	С	412	LEU
1	D	25	TYR



Mol	Chain	Res	Type
1	D	38	ILE
1	D	91	LEU
1	D	132	VAL
1	D	144	LYS
1	D	179	ARG
1	D	228	ASP
1	D	292	HIS
1	D	301	TYR
1	D	334	LEU
1	D	335	ILE
1	D	385	PHE
1	D	406	LYS

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 21 ligands modelled in this entry, 15 are monoatomic - leaving 6 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).



Mal	Turne	Chain	Dec	Tink	Bo	ond leng	$_{\rm ths}$	B	ond ang	les
IVIOI	Type	Unam	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
5	144	С	505	-	1,7,7	1.24	0	3,9,9	0.05	0
5	144	D	506	-	1,7,7	1.23	0	3,9,9	0.11	0
4	4VX	В	505	2	25,33,33	0.60	0	25,48,48	0.83	1 (4%)
4	4VX	D	505	-	25,33,33	0.60	0	25,48,48	0.89	2 (8%)
4	4VX	А	504	-	25,33,33	0.59	0	25,48,48	0.86	1 (4%)
4	4VX	С	504	2	25,33,33	0.61	0	25,48,48	0.85	1 (4%)

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
5	144	С	505	-	-	0/0/9/9	-
5	144	D	506	-	-	0/0/9/9	-
4	4VX	В	505	2	-	3/10/22/22	0/5/5/5
4	4VX	D	505	-	-	2/10/22/22	0/5/5/5
4	4VX	А	504	-	-	2/10/22/22	0/5/5/5
4	4VX	С	504	2	-	2/10/22/22	0/5/5/5

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
4	D	505	4VX	C8-C6-C5	-3.18	105.52	114.39
4	А	504	4VX	C8-C6-C5	-3.17	105.55	114.39
4	В	505	4VX	C8-C6-C5	-3.16	105.58	114.39
4	С	504	4VX	C8-C6-C5	-3.16	105.58	114.39
4	D	505	4VX	C13-C16-N2	2.01	118.70	115.48

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	В	505	4VX	N1-C11-C12-C15
4	В	505	4VX	C12-C11-N1-C7
4	С	504	4VX	C12-C11-N1-C7
4	А	504	4VX	С9-С10-С17-С18
4	D	505	4VX	C9-C10-C17-C22



Mol	Chain	Res	Type	Atoms
4	В	505	4VX	C12-C11-N1-C5
4	С	504	4VX	C12-C11-N1-C5
4	А	504	4VX	C9-C10-C17-C22
4	D	505	4VX	С9-С10-С17-С18

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	С	505	144	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.













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, 95^{th} 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	А	402/440~(91%)	0.81	38~(9%) 8	11		37, 47, 58, 65	0
1	В	406/440~(92%)	0.92	61 (15%) 2	2 3		34, 47, 55, 61	0
1	С	409/440~(92%)	1.31	94 (22%) 0) 1		41, 51, 62, 68	0
1	D	374/440~(85%)	1.23	82 (21%) 0) 1		43, 53, 60, 63	0
All	All	1591/1760~(90%)	1.06	275 (17%) 1	1	1	34, 50, 60, 68	0

All (275) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	287	LEU	11.3
1	С	265	ILE	8.2
1	С	272	VAL	8.1
1	D	271	ILE	7.3
1	С	346	THR	7.0
1	D	59	VAL	6.7
1	С	252	GLY	6.5
1	С	336	LEU	6.1
1	С	70	ALA	6.0
1	А	425	ILE	5.8
1	А	432	TYR	5.6
1	D	67	TYR	5.5
1	С	204	VAL	5.5
1	В	279	VAL	5.5
1	В	326	ILE	5.5
1	D	21	PHE	5.4
1	С	300	PHE	5.3
1	D	187	LEU	5.2
1	В	425	ILE	5.0
1	В	435	TYR	5.0
1	С	98	ASN	4.8



Mol	Chain	Res	Type	RSRZ
1	D	92	MET	4.8
1	В	346	THR	4.8
1	С	211	ALA	4.8
1	В	21	PHE	4.7
1	С	14	LEU	4.7
1	С	182	TYR	4.7
1	С	151	PHE	4.7
1	С	334	LEU	4.7
1	D	284	ALA	4.7
1	D	68	VAL	4.6
1	С	253	ILE	4.6
1	А	95	PHE	4.5
1	D	105	PRO	4.4
1	В	424	LEU	4.4
1	С	154	LEU	4.3
1	С	108	PHE	4.3
1	В	73	LYS	4.2
1	С	302	PRO	4.1
1	А	32	ILE	4.1
1	D	282	CYS	4.1
1	С	56	TYR	4.1
1	D	404	ILE	4.1
1	С	387	LEU	4.1
1	В	252	GLY	4.0
1	D	336	LEU	4.0
1	В	237	ALA	4.0
1	С	11	TYR	4.0
1	D	225	VAL	4.0
1	В	182	TYR	4.0
1	В	106	SER	4.0
1	В	387	LEU	3.9
1	D	281	GLN	3.9
1	В	282[A]	CYS	3.9
1	А	99	TYR	3.8
1	А	428	TYR	3.8
1	А	287	LEU	3.8
1	А	356	LEU	3.8
1	В	271	ILE	3.8
1	С	97	LEU	3.8
1	А	271	ILE	3.7
1	А	219	THR	3.7
1	С	294	ILE	3.7



Mol	Chain	Res	Type	RSRZ
1	С	155	ASN	3.7
1	С	310	CYS	3.7
1	С	196	ALA	3.7
1	В	428	TYR	3.7
1	D	41	LEU	3.6
1	С	21	PHE	3.6
1	D	110	TYR	3.6
1	D	320	LEU	3.6
1	С	198	TRP	3.6
1	В	389	ILE	3.6
1	D	262	ILE	3.6
1	С	119	LEU	3.5
1	В	297	LEU	3.5
1	С	115	VAL	3.5
1	С	298	THR	3.5
1	А	92	MET	3.4
1	D	134	ILE	3.4
1	D	275	PRO	3.4
1	В	269	LEU	3.4
1	А	426	TYR	3.4
1	D	288	ALA	3.3
1	D	104	PHE	3.3
1	С	404	ILE	3.3
1	С	231	PRO	3.3
1	С	303	ASN	3.3
1	А	122	ALA	3.3
1	D	165	VAL	3.3
1	С	65	THR	3.2
1	D	327	LEU	3.2
1	С	99	TYR	3.2
1	B	336	LEU	3.2
1	C	264	PRO	3.2
1	D	77	LEU	3.2
1	D	34	ALA	3.2
1	D	70	ALA	3.2
1	D	289	THR	3.1
1	С	68	VAL	3.1
1	В	426	TYR	3.1
1	D	426	TYR	3.1
1	D	286	CYS	3.1
1	D	268	SER	3.1
1	А	185	LEU	3.1



Mol	Chain	Res	Type	RSRZ
1	В	345	ASP	3.1
1	С	73	LYS	3.0
1	С	318	GLY	3.0
1	D	90	LEU	3.0
1	С	183	VAL	3.0
1	D	258	TRP	3.0
1	А	300	PHE	3.0
1	С	130	CYS	3.0
1	С	415	LEU	3.0
1	С	126	ILE	3.0
1	С	319	TYR	2.9
1	С	86	ALA	2.9
1	D	89	GLU	2.9
1	В	159	LEU	2.9
1	С	106	SER	2.9
1	А	132	VAL	2.9
1	В	198	TRP	2.9
1	С	218	GLY	2.9
1	D	296	ARG	2.9
1	А	62	PHE	2.9
1	С	59	VAL	2.9
1	D	318	GLY	2.9
1	D	266	LEU	2.9
1	В	230	LEU	2.9
1	С	345	ASP	2.8
1	D	153	TYR	2.8
1	А	326	ILE	2.8
1	D	25	TYR	2.8
1	В	272	VAL	2.8
1	В	181	LEU	2.8
1	С	139	GLY	2.8
1	С	107	VAL	2.8
1	В	268	SER	2.8
1	С	238	GLY	2.8
1	С	221	THR	2.7
1	С	246	ASN	2.7
1	С	349	LEU	2.7
1	D	256	LEU 2.7	
1	D	298	THR	2.7
1	С	271	ILE	2.7
1	D	199[A]	TYR	2.7
1	C	26	ALA	2.7



Mol	Chain	Res	Type RSR2	
1	В	71	LEU	2.7
1	С	77	LEU	2.7
1	А	282[A]	CYS	2.7
1	В	199	TYR	2.7
1	D	351	THR	2.7
1	С	292	HIS	2.6
1	В	296	ARG	2.6
1	D	27	LEU	2.6
1	D	425	ILE	2.6
1	С	31	LEU	2.6
1	А	49	TRP	2.6
1	D	161	ILE	2.6
1	В	56	TYR	2.6
1	А	70	ALA	2.6
1	С	247	LEU	2.6
1	С	28	VAL	2.6
1	С	76	MET	2.6
1	D	28	VAL	2.6
1	В	347	ALA	2.6
1	С	205	THR	2.5
1	С	329	TRP	2.5
1	D	349	LEU	2.5
1	С	394	HIS	2.5
1	В	265	ILE	2.5
1	А	404	ILE	2.5
1	В	322	ALA	2.5
1	С	322	ALA	2.5
1	D	91	LEU	2.5
1	D	361	VAL	2.5
1	А	182	TYR	2.5
1	С	413	GLU	2.5
1	А	105	PRO	2.5
1	D	207	SER	2.4
1	С	34	ALA	2.4
1	С	361	VAL	2.4
1	A	382	GLY	2.4
1	A	119	LEU	2.4
1	В	77	LEU	2.4
1	В	329	TRP	2.4
1	С	377	TYR	2.4
1	D	32	ILE	2.4
1	D	197	PHE	2.4



Mol	Chain	Res	Res Type	
1	D	385	PHE	2.4
1	С	181	LEU	2.4
1	С	284	ALA	2.4
1	В	280	VAL	2.4
1	D	178	THR	2.4
1	С	396	SER	2.4
1	В	412	LEU	2.4
1	А	262	ILE	2.3
1	В	258	TRP	2.3
1	D	218	GLY	2.3
1	С	153	TYR	2.3
1	В	26	ALA	2.3
1	D	347	ALA	2.3
1	В	49	TRP	2.3
1	С	224	MET	2.3
1	D	146	SER	2.3
1	В	151	PHE	2.3
1	А	7	TYR	2.3
1	D	112	LEU	2.3
1	D	355	ALA	2.3
1	D	356	LEU	2.3
1	В	2	SER	2.3
1	С	317	SER	2.3
1	С	44	VAL	2.3
1	В	99	TYR	2.3
1	В	289	THR	2.3
1	В	320	LEU	2.3
1	С	25	TYR	2.3
1	D	219	THR	2.3
1	В	382	GLY	2.3
1	В	249	LEU	2.2
1	В	319	TYR	2.2
1	В	248	PRO	2.2
1	С	32	ILE	2.2
1	D	148	ALA	2.2
1	D	260	ASN	2.2
1	С	165	VAL	2.2
1	А	97	LEU	2.2
1	С	391	TYR	2.2
1	C	291	PRO	2.2
1	В	153	TYR	2.2
1	D	276	SER	2.2



Mol	Chain	Res	Type	RSRZ
1	D	252	GLY	2.2
1	D	86	ALA	2.2
1	D	124	ALA	2.2
1	С	92	MET	2.2
1	А	373	PRO	2.2
1	В	65	THR	2.2
1	D	71	LEU	2.2
1	С	75	GLN	2.2
1	А	67	TYR	2.1
1	А	331	VAL	2.1
1	С	180	VAL	2.1
1	С	27	LEU	2.1
1	D	269	LEU	2.1
1	А	47	LEU	2.1
1	С	230	LEU	2.1
1	D	4	GLY	2.1
1	С	316	LEU	2.1
1	D	302	PRO	2.1
1	В	350	TRP	2.1
1	А	391	TYR	2.1
1	В	143	ALA	2.1
1	С	320	LEU	2.1
1	D	190	GLY	2.1
1	А	421	LEU	2.1
1	В	292	HIS	2.1
1	D	407	HIS	2.1
1	С	101	CYS	2.1
1	С	350	TRP	2.1
1	А	199	TYR	2.1
1	D	182	TYR	2.1
1	D	428	TYR	2.1
1	A	336	LEU	2.0
1	В	253	ILE	2.0
1	В	295	PHE	2.0
1	D	140	TRP	2.0
1	D	216	PHE	2.0
1	D	410	ARG	2.0
1	В	349	LEU	2.0
1	D	139	GLY	2.0
1	В	86	ALA	2.0
1	С	376	SER	2.0
1	А	100	ASP	2.0



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Mol	Chain	\mathbf{Res}	Type	RSRZ	
1	D	280	VAL	2.0	
1	В	432	TYR	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, 95^{th} 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
4	4VX	А	504	29/29	0.68	0.20	$63,\!65,\!66,\!68$	0
4	4VX	С	504	29/29	0.71	0.23	77,78,79,79	0
4	4VX	D	505	29/29	0.74	0.23	60,62,63,64	0
3	K	В	503	1/1	0.75	0.22	73,73,73,73	0
3	K	С	503	1/1	0.78	0.10	59, 59, 59, 59, 59	0
4	4VX	В	505	29/29	0.83	0.17	$63,\!63,\!65,\!68$	0
5	144	D	506	8/8	0.84	0.17	44,44,44,44	0
3	K	В	504	1/1	0.85	0.15	119,119,119,119	0
3	K	D	502	1/1	0.87	0.20	59, 59, 59, 59	0
6	CL	D	504	1/1	0.88	0.23	41,41,41,41	1
3	K	D	503	1/1	0.90	0.12	67,67,67,67	0
3	K	С	502	1/1	0.94	0.06	52,52,52,52	0
2	ZN	С	501	1/1	0.94	0.12	48,48,48,48	0
5	144	С	505	8/8	0.95	0.16	48,48,48,49	0
2	ZN	В	501	1/1	0.96	0.10	46,46,46,46	0
3	K	С	506	1/1	0.97	0.10	37,37,37,37	1
3	K	А	503	1/1	0.97	0.12	58,58,58,58	0
3	K	В	502	1/1	0.98	0.06	44,44,44,44	0
3	K	А	502	1/1	0.98	0.05	42,42,42,42	0
2	ZN	D	501	1/1	0.98	0.02	54,54,54,54	0
2	ZN	А	501	1/1	0.99	0.08	41,41,41,41	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.















6.5 Other polymers (i)

There are no such residues in this entry.

