

Full wwPDB X-ray Structure Validation Report (i)

Oct 14, 2023 – 01:57 PM EDT

:	8D94
:	SAMHD1-DNA complex
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:	2022-06-09
:	2.44 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
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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

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 2.44 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\text{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617(2.46-2.42)
Sidechain outliers	138945	1617(2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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					
			3%					
1	А	626	60%	11%	29%			
			3%					
1	В	626	61%	8%	31%			
			<u>2</u> %					
1	С	626	62%	10%	27%			
			3%					
1	D	626	57%	12%	31%			
			40%					
2	F	5	60%		40%			



α \cdot \cdot \cdot	C		
Continued	trom	previous	page
	9	1	1 0

Mol	Chain	Length		Quality of ch	ain
			20%		
2	G	5	40%	20%	40%
_					
2	Н	5	40%		60%
			20%		
2	Ι	5	20%	40%	40%



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 14917 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	Δ	447	Total	С	Ν	0	S	0	0	0
1	А	441	3616	2319	624	654	19	0	0	0
1	р	424	Total	С	Ν	0	S	0	0	0
1	ГВ	404	3521	2258	611	633	19	0	0	U
1	С	455	Total	С	Ν	0	S	0	0	0
1	U	400	3668	2348	631	669	20	0		0
1	1 D	421	Total	С	Ν	0	S	0	0	0
	D	401	3484	2234	606	625	19	0	0	0

• Molecule 1 is a protein called Deoxynucleoside triphosphate triphosphohydrolase SAMHD1.

• Molecule 2 is a DNA chain called DNA (5'-D(P*TP*GP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	2 F	3	Total	С	Ν	Ο	Р	0	0	0
		5	62	30	9	20	3	0	0	
9	C	G 3	Total	С	Ν	Ο	Р	0	0	0
	2 G		62	30	9	20	3	0		
0	ц	2	Total	С	Ν	0	Р	0	0	0
	H		42	20	7	13	2	0		0
0	о I	2	Total	С	Ν	Ο	Р	0	0	0
	3	62	30	9	20	3	0		0	

• Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total Fe 1 1	0	0
3	В	1	Total Fe 1 1	0	0
3	С	1	Total Fe 1 1	0	0
3	D	1	Total Fe 1 1	0	0



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- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	Total Ca 1 1	0	0
4	В	1	Total Ca 1 1	0	0
4	С	1	Total Ca 1 1	0	0
4	D	1	Total Ca 1 1	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	111	Total O 111 111	0	0
5	В	80	Total O 80 80	0	0
5	С	117	Total O 117 117	0	0
5	D	82	TotalO8282	0	0
5	F	1	Total O 1 1	0	0
5	G	1	Total O 1 1	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.











K486 V487 L488 L489 D490 V491 V491 M505	ASP TYR GLY GLY GLU GLU CLV GLU FLV FLC TLE ILE ILE	V518 5529 7520 7521 7524 7523 7523 7523 8523 7524 7523 7524 7523 7524 7523 7524 7523 7524 7523 7524 7524 7524 7524 7527 7527 7527 7527	AKG THR LYS ASN ASN ASN ALN GLN GLN CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	K556 V557 D558 R559
K560 S561 L562 L562 L562 F573 F578 F578 F578 F581 F581 F581 F581	D583 GLY ASP VAL ALA ALA PLC LLEU LLEU LLEU TLE PRO FLN GLN	LYS LYS GLU GLU ASN ASN ASN SER SER CAL ASN ASN	ARA ARG ARG ARG ARG ARG ALA ARA ARA CAN CAN CAN CAN CAN CAN CAN CAN CAN CA	
• Molecule 2:	DNA (5'-D(P*7	CP*GP*T)-3')		
Chain F:	40% 60%	6	40%	
DC DA G3 G3 T4				
• Molecule 2:	DNA (5'-D(P*1	TP*GP*T)-3')		
Chain G:	20% 40%	20%	40%	
DC DA T2 G3 T4				
• Molecule 2:	DNA (5'-D(P*7	TP*GP*T)-3')		
Chain H:	40%		60%	
DC DA 14 14				
• Molecule 2:	DNA (5'-D(P*7	TP*GP*T)-3')		
Chain I:	20%	40%	40%	
DC 12 33 44				



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	75.12Å 179.94Å 79.79Å	Depositor
a, b, c, α , β , γ	90.00° 108.95° 90.00°	Depositor
Bosolution(A)	38.98 - 2.44	Depositor
Resolution (A)	38.98 - 2.44	EDS
% Data completeness	87.5 (38.98-2.44)	Depositor
(in resolution range)	87.5 (38.98-2.44)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.51 (at 2.45 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
D D.	0.190 , 0.243	Depositor
n, n_{free}	0.190 , 0.245	DCC
R_{free} test set	1978 reflections (3.05%)	wwPDB-VP
Wilson B-factor $(Å^2)$	41.1	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent $k_{sol}(e/A^3)$, $B_{sol}(A^2)$	0.32 , 52.2	EDS
L-test for twinning ²	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14917	wwPDB-VP
Average B, all atoms $(Å^2)$	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.28% 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: FE, CA

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	Bond lengths		angles
IVIOI		RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.25	0/3702	0.47	0/5002
1	В	0.24	0/3604	0.46	0/4865
1	С	0.24	0/3756	0.45	0/5078
1	D	0.24	0/3566	0.47	0/4817
2	F	0.51	0/68	1.11	0/103
2	G	0.58	0/68	1.17	0/103
2	Н	0.51	0/46	1.01	0/69
2	Ι	0.53	0/68	1.15	0/103
All	All	0.25	0/14878	0.48	0/20140

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	3616	0	3540	45	0
1	В	3521	0	3461	36	0
1	С	3668	0	3564	42	0
1	D	3484	0	3410	49	0
2	F	62	0	36	6	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	62	0	36	4	0
2	Н	42	0	24	6	0
2	Ι	62	0	36	3	0
3	А	1	0	0	0	0
3	В	1	0	0	0	0
3	С	1	0	0	0	0
3	D	1	0	0	0	0
4	А	1	0	0	0	0
4	В	1	0	0	0	0
4	С	1	0	0	0	0
4	D	1	0	0	0	0
5	А	111	0	0	5	0
5	В	80	0	0	1	0
5	С	117	0	0	3	0
5	D	82	0	0	7	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
All	All	14917	0	14107	170	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 6.

All (170) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:238:VAL:HG13	1:B:269:LYS:HD3	1.68	0.76
1:B:117:VAL:HG13	2:H:4:DT:H5"	1.69	0.74
1:A:378:VAL:HG11	2:F:3:DG:H5"	1.75	0.68
1:D:476:LEU:HD23	1:D:500:VAL:HG11	1.76	0.68
1:D:462:PRO:HG3	1:D:548:GLN:HE21	1.58	0.67
1:C:269:LYS:NZ	5:C:804:HOH:O	2.31	0.64
1:A:372:ARG:HE	2:F:4:DT:H3	1.45	0.63
1:D:577:ASN:ND2	5:D:804:HOH:O	2.31	0.63
1:C:583:ASP:OD1	1:C:583:ASP:N	2.33	0.62
1:B:359:LEU:HD11	1:B:518:VAL:HG21	1.83	0.61
1:A:372:ARG:NH1	5:A:801:HOH:O	2.15	0.61
1:C:199:VAL:HA	1:C:271:GLN:HE22	1.66	0.61
1:A:326:GLN:H	1:A:326:GLN:CD	2.04	0.60
1:B:155:TYR:O	1:B:451:ARG:NH2	2.34	0.60
1:C:465:GLN:NE2	5:C:807:HOH:O	2.35	0.59
1:D:216:MET:SD	1:D:387:THR:OG1	2.60	0.59



	A L O	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:A:116:LYS:NZ	2:I:2:DT:O3'	2.36	0.59	
2:H:3:DG:N2	2:H:3:DG:OP1	2.35	0.59	
1:D:254:MET:HG2	1:D:259:LEU:HD12	1.86	0.58	
1:B:566:ARG:NH2	1:B:582:GLN:O	2.36	0.57	
1:C:465:GLN:OE1	1:C:577:ASN:ND2	2.34	0.57	
1:B:326:GLN:NE2	1:D:326:GLN:OE1	2.37	0.57	
1:A:343:VAL:HG22	1:A:529:ALA:HB2	1.87	0.57	
1:A:523:LYS:HE3	1:A:524:THR:HG22	1.87	0.57	
1:A:220:ARG:HG2	1:A:387:THR:HG21	1.86	0.57	
1:D:155:TYR:O	1:D:451:ARG:NH2	2.35	0.56	
1:C:116:LYS:NZ	2:G:3:DG:OP1	2.26	0.56	
1:A:191:ILE:HD11	1:A:296:PHE:HE2	1.69	0.56	
1:C:451:ARG:HG2	2:H:3:DG:N2	2.20	0.56	
1:D:146:TYR:OH	5:D:801:HOH:O	2.17	0.56	
1:D:500:VAL:HG22	1:D:552:VAL:HG22	1.86	0.56	
1:B:439:LYS:O	1:B:443:GLU:HG2	2.05	0.56	
1:B:425:ASN:ND2	1:C:425:ASN:OD1	2.39	0.56	
1:D:114:THR:HB	1:D:130:PRO:HG3	1.87	0.55	
1:B:425:ASN:HB2	1:C:428:LEU:HD13	1.89	0.54	
1:D:340:VAL:HG12	1:D:347:LEU:HD12	1.89	0.54	
1:D:455:LYS:HG3	1:D:562:LEU:HD11	1.88	0.54	
1:D:370:HIS:O	1:D:375:GLN:HG3	2.07	0.54	
1:B:580:LYS:HD2	1:B:581:PRO:HD2	1.88	0.54	
1:C:155:TYR:HB3	1:C:451:ARG:HH22	1.72	0.54	
1:D:167:HIS:ND1	1:D:314:ASP:OD2	2.37	0.53	
1:A:155:TYR:HB3	1:A:451:ARG:HH22	1.73	0.53	
1:A:195:ASP:OD2	1:A:294:LYS:NZ	2.32	0.53	
1:B:175:ALA:HB1	1:B:199:VAL:HG12	1.90	0.53	
1:B:494:LYS:HD3	1:B:496:GLU:HB3	1.91	0.53	
1:C:115:MET:HE2	1:C:127:GLU:HB3	1.91	0.53	
1:C:132:LEU:HD22	1:C:204:LEU:HD22	1.90	0.53	
1:A:370:HIS:HA	1:A:374:TYR:HB2	1.91	0.52	
1:D:412:ALA:HB3	1:D:422:LEU:HD22	1.91	0.52	
1:D:446:LYS:NZ	5:D:810:HOH:O	2.43	0.51	
1:A:394:ASP:O	1:A:408:ARG:HD2	2.10	0.51	
1:A:405:LYS:HD2	1:A:407:TYR:CZ	2.46	0.51	
1:D:378:VAL:HG11	2:I:3:DG:H5'	1.93	0.51	
1:B:485:PRO:HG2	1:B:489:LEU:HD11	1.93	0.50	
1:A:543:GLU:N	1:A:543:GLU:OE1	2.44	0.50	
1:D:468:ILE:H	1:D:548:GLN:HE22	1.58	0.50	
1:D:306:ASN:HB2	1:D:308:ILE:HG22	1.92	0.50	



Interatomic Clash					
Atom-1	Atom-2	distance (Å)	overlap (Å)		
1:A:468:ILE:HG21	1:A:476:LEU:HD11	1.94	0.50		
1:C:148:LYS:O	1:C:214:SER:OG	2.25	0.49		
1:A:459:GLU:HG3	1:A:551:ARG:HG2	1.93	0.49		
1:B:299:GLU:OE1	1:B:348:ARG:HB2	2.13	0.49		
1:C:129:HIS:HD2	1:C:131:LEU:H	1.61	0.49		
1:C:366:ARG:NH1	1:C:545:PHE:HE1	2.11	0.49		
1:B:378:VAL:HG21	2:G:3:DG:H5"	1.94	0.49		
1:C:372:ARG:HE	2:H:4:DT:H3	1.60	0.49		
1:A:185:LYS:NZ	5:A:809:HOH:O	2.33	0.48		
1:C:370:HIS:HA	1:C:374:TYR:HB2	1.95	0.48		
1:D:560:LYS:HD2	1:D:560:LYS:HA	1.66	0.48		
1:A:155:TYR:HB3	1:A:451:ARG:NH2	2.29	0.48		
1:C:129:HIS:CD2	1:C:131:LEU:H	2.32	0.48		
1:C:392:LYS:HD3	1:C:440:ASP:HB3	1.95	0.48		
1:C:276:LEU:HD12	1:C:277:GLU:HG3	1.94	0.48		
1:B:494:LYS:HD3	1:B:496:GLU:H	1.79	0.48		
1:D:264:ASP:O	1:D:268:ILE:HG12	2.14	0.48		
1:B:372:ARG:NH2	1:D:361:ASP:OD2	2.41	0.47		
1:A:372:ARG:NH2	5:A:801:HOH:O	2.47	0.47		
1:D:558:ASP:OD2	1:D:561:SER:N	2.47	0.47		
1:A:309:ASP:OD1	1:A:312:LYS:HG2	2.15	0.47		
1:D:117:VAL:HG22	1:D:127:GLU:HG2	1.95	0.47		
1:D:485:PRO:HG2	1:D:489:LEU:HD11	1.97	0.47		
1:A:435:ASP:O	1:A:442:ARG:NH2	2.46	0.47		
1:B:167:HIS:ND1	1:B:314:ASP:OD2	2.48	0.47		
1:C:175:ALA:HB1	1:C:199:VAL:HG12	1.96	0.47		
1:B:288:LYS:HA	1:B:288:LYS:HD2	1.76	0.46		
1:D:189:LEU:HD12	1:D:296:PHE:CZ	2.50	0.46		
1:C:378:VAL:HG11	2:H:3:DG:H5'	1.96	0.46		
1:C:150:LEU:HD12	1:C:160:ALA:HB1	1.96	0.46		
1:C:506:ASP:N	1:C:506:ASP:OD1	2.46	0.46		
1:C:190:GLN:O	1:C:294:LYS:NZ	2.49	0.46		
1:B:118:ILE:HD13	2:H:3:DG:H2"	1.97	0.46		
1:C:143:ARG:HD2	1:C:420:THR:HA	1.97	0.46		
1:A:353:ASP:OD2	1:A:522:CYS:HA	2.15	0.46		
1:D:116:LYS:HE3	2:F:3:DG:OP1	2.16	0.46		
1:C:202:ALA:HB3	1:C:271:GLN:HE21	1.81	0.46		
1:D:188:GLU:HG2	1:D:189:LEU:HD22	1.97	0.45		
1:D:306:ASN:CB	1:D:308:ILE:HG22	2.46	0.45		
1:D:302:SER:O	5:D:802:HOH:O	2.21	0.45		
1:D:337:PHE:HD1	1:D:352:ARG:HB2	1.80	0.45		



Interatomic C					
Atom-1	Atom-2	distance (Å)	overlap (Å)		
1:A:267:PHE:O	1:A:271:GLN:HG2	2.15	0.45		
1:B:451:ARG:NH1	5:B:802:HOH:O	2.37	0.45		
1:B:343:VAL:HG21	1:B:519:SER:HB2	1.99	0.45		
1:B:326:GLN:NE2	1:D:328:ASN:HD22	2.15	0.45		
1:C:408:ARG:H	1:C:411:THR:HG1	1.65	0.45		
1:C:496:GLU:H	1:C:496:GLU:HG2	1.59	0.45		
1:D:435:ASP:O	1:D:442:ARG:NH2	2.50	0.45		
1:A:250:ILE:O	1:A:254:MET:HG3	2.17	0.44		
1:A:333:ARG:HB3	1:A:355:GLU:OE1	2.18	0.44		
1:A:500:VAL:HG22	1:A:552:VAL:HG22	1.99	0.44		
1:D:118:ILE:HD11	2:F:3:DG:C8	2.52	0.44		
2:F:2:DT:H2"	2:F:3:DG:O5'	2.15	0.44		
1:B:412:ALA:HB3	1:B:422:LEU:HD22	1.98	0.44		
1:D:556:LYS:HE2	1:D:561:SER:OG	2.17	0.44		
1:A:575:ASP:OD1	1:A:575:ASP:N	2.50	0.44		
1:C:343:VAL:HG22	1:C:529:ALA:HB2	2.00	0.44		
1:A:178:LEU:HA	1:A:335:ILE:HG23	1.99	0.44		
1:B:169:LEU:HD23	1:B:204:LEU:HD11	2.00	0.44		
1:D:352:ARG:NH2	5:D:814:HOH:O	2.48	0.44		
1:B:312:LYS:HA	1:B:315:TYR:CE2	2.53	0.44		
1:D:241:PHE:CZ	1:D:245:ILE:HD11	2.53	0.44		
1:A:175:ALA:HB1	1:A:199:VAL:HG12	1.99	0.43		
1:A:339:ARG:HD3	1:A:526:PRO:O	2.18	0.43		
1:C:456:TYR:HE1	1:C:551:ARG:HD3	1.82	0.43		
1:C:505:MET:HE3	1:C:546:ALA:H	1.82	0.43		
1:B:118:ILE:HB	1:B:126:ILE:HG13	2.00	0.43		
1:C:498:PHE:HZ	1:C:568:TYR:HD1	1.67	0.43		
1:A:456:TYR:OH	1:A:459:GLU:HB2	2.18	0.43		
1:C:505:MET:HG3	1:C:547:GLU:HA	1.99	0.43		
1:D:255:GLU:OE1	5:D:803:HOH:O	2.21	0.43		
1:D:189:LEU:C	1:D:190:GLN:HG2	2.39	0.43		
1:A:157:PHE:CE2	2:F:4:DT:H2"	2.54	0.42		
1:A:367:ASN:ND2	1:A:543:GLU:HB3	2.34	0.42		
1:C:199:VAL:HA	1:C:271:GLN:NE2	2.33	0.42		
1:A:312:LYS:HD3	1:A:315:TYR:OH	2.20	0.42		
1:A:118:ILE:HD11	2:I:3:DG:C8	2.55	0.42		
1:A:399:ILE:HD11	1:A:426:ILE:HD11	2.01	0.42		
1:A:212:PRO:HD2	1:A:217:PHE:CD1	2.55	0.42		
1:B:463:THR:C	1:B:465:GLN:H	2.23	0.42		
1:C:427:PHE:CE2	1:C:445:LEU:HD22	2.54	0.42		
1:B:316:PHE:CZ	1:B:366:ARG:HB2	2.55	0.42		



	A + 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:367:ASN:HD21	1:A:543:GLU:HB3	1.85	0.42
1:B:427:PHE:CE2	1:B:445:LEU:HD22	2.55	0.42
1:C:490:ASP:OD1	1:C:490:ASP:N	2.42	0.42
1:D:155:TYR:HB3	1:D:451:ARG:NH2	2.34	0.42
1:A:136:ILE:HG13	1:A:204:LEU:HD21	2.02	0.41
1:C:155:TYR:O	1:C:451:ARG:NH2	2.53	0.41
1:C:366:ARG:NH1	5:C:824:HOH:O	2.53	0.41
1:B:313:TRP:HA	1:B:316:PHE:HB2	2.01	0.41
1:D:129:HIS:N	5:D:817:HOH:O	2.53	0.41
1:D:467:LYS:O	1:D:469:LYS:HE3	2.20	0.41
1:A:299:GLU:OE2	1:A:348:ARG:HG2	2.21	0.41
1:B:339:ARG:NH1	1:B:526:PRO:HB3	2.36	0.41
1:B:346:GLU:HB3	1:B:348:ARG:NH2	2.36	0.41
2:G:3:DG:H2'	2:G:3:DG:N3	2.35	0.41
1:B:443:GLU:O	1:B:447:GLN:HG2	2.20	0.41
1:D:182:LEU:HD22	1:D:340:VAL:HG23	2.02	0.41
1:D:226:ARG:CZ	1:D:229:VAL:HG21	2.51	0.41
1:D:228:GLU:OE2	1:D:228:GLU:N	2.31	0.41
1:A:312:LYS:NZ	5:A:819:HOH:O	2.53	0.41
1:B:451:ARG:HG2	2:G:3:DG:N2	2.35	0.41
1:D:427:PHE:CE2	1:D:445:LEU:HD22	2.56	0.41
1:A:254:MET:HG3	1:A:254:MET:H	1.74	0.41
1:D:474:GLU:O	1:D:477:PRO:HD2	2.20	0.41
1:A:352:ARG:HB3	1:A:355:GLU:HG2	2.02	0.41
1:C:134:ARG:HG3	1:C:253:VAL:HG11	2.03	0.41
1:D:269:LYS:O	1:D:273:VAL:HG12	2.22	0.41
1:C:367:ASN:HB2	1:C:543:GLU:OE2	2.22	0.40
1:A:333:ARG:NH1	5:A:817:HOH:O	2.50	0.40
1:B:382:ILE:O	1:B:386:ILE:HG13	2.22	0.40
1:C:118:ILE:O	1:C:126:ILE:HG12	2.21	0.40
1:D:197:LEU:HD12	1:D:197:LEU:HA	1.86	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.



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	А	439/626~(70%)	426~(97%)	12 (3%)	1 (0%)	47 57
1	В	426/626~(68%)	414 (97%)	12 (3%)	0	100 100
1	С	449/626~(72%)	434~(97%)	15 (3%)	0	100 100
1	D	423/626~(68%)	414 (98%)	9~(2%)	0	100 100
All	All	1737/2504~(69%)	1688 (97%)	48 (3%)	1 (0%)	51 64

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

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	542	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	Percentile	\mathbf{s}
1	А	385/560~(69%)	378~(98%)	7(2%)	59 71	
1	В	376/560~(67%)	369~(98%)	7 (2%)	57 69	
1	С	389/560~(70%)	383~(98%)	6 (2%)	65 76	
1	D	370/560~(66%)	366~(99%)	4 (1%)	73 83	
All	All	1520/2240 (68%)	1496 (98%)	24 (2%)	62 74	

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	371	ARG
1	А	451	ARG
1	А	492	LYS
1	А	506	ASP
1	А	523	LYS
1	А	547	GLU
1	А	549	LEU



Mol	Chain	Res	Type
1	В	194	ARG
1	В	263	GLU
1	В	316	PHE
1	В	405	LYS
1	В	451	ARG
1	В	465	GLN
1	В	505	MET
1	С	185	LYS
1	С	451	ARG
1	С	478	LYS
1	С	544	LYS
1	С	557	VAL
1	С	559	ARG
1	D	328	ASN
1	D	336	LYS
1	D	366	ARG
1	D	582	GLN

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

Mol	Chain	Res	Type
1	В	326	GLN
1	В	425	ASN
1	В	447	GLN
1	С	271	GLN
1	D	375	GLN
1	D	548	GLN

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 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis. There are no bond length outliers. There are no bond angle outliers. There are no chirality outliers. There are no torsion outliers. There are no ring outliers. No monomer is involved in short contacts.

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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	$Q{<}0.9$
1	А	447/626~(71%)	0.03	17 (3%) 40 37	24, 41, 87, 114	0
1	В	434/626~(69%)	0.03	18 (4%) 37 34	27, 46, 93, 117	0
1	С	455/626~(72%)	0.02	14 (3%) 49 45	25, 45, 83, 109	0
1	D	431/626~(68%)	0.14	21 (4%) 29 27	28, 47, 89, 114	0
2	F	3/5~(60%)	3.90	2(66%) 0 0	63, 63, 64, 77	3 (100%)
2	G	3/5~(60%)	1.68	1 (33%) 0 0	51, 51, 59, 80	3 (100%)
2	Н	2/5~(40%)	1.32	0 100 100	55, 55, 55, 60	2(100%)
2	Ι	3/5~(60%)	1.99	1 (33%) 0 0	56, 56, 58, 90	3 (100%)
All	All	1778/2524 (70%)	0.07	74 (4%) 36 33	24, 45, 88, 117	11 (0%)

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	2	DT	6.7
1	D	522	CYS	5.7
1	С	491	VAL	5.0
1	D	518	VAL	4.6
1	D	466	ILE	4.6
1	D	114	THR	4.6
1	В	489	LEU	4.4
1	А	114	THR	4.1
1	В	517	HIS	4.1
1	В	516	ASP	4.0
1	D	329	PHE	3.9
1	А	545	PHE	3.9
1	А	284	LEU	3.9
2	Ι	2	DT	3.8
1	А	544	LYS	3.6
1	С	487	VAL	3.5



1

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\mathbf{Mol}	Chain	\mathbf{Res}	Type	RSRZ	

485

PRO

3.4

D

1	А	360	TYR	3.4
1	А	542	PRO	3.4
1	В	115	MET	3.3
1	D	582	GLN	3.2
1	В	524	THR	3.2
1	С	488	LEU	3.2
2	F	4	DT	3.1
1	А	541	LEU	3.1
1	С	489	LEU	3.1
1	А	583	ASP	3.1
1	А	515	ILE	3.0
1	С	114	THR	3.0
2	G	2	DT	3.0
1	В	334	PHE	3.0
1	С	524	THR	2.9
1	А	526	PRO	2.9
1	D	488	LEU	2.9
1	D	353	ASP	2.9
1	В	525	ALA	2.8
1	В	464	GLY	2.7
1	D	581	PRO	2.7
1	D	352	ARG	2.6
1	D	489	LEU	2.6
1	D	517	HIS	2.6
1	С	545	PHE	2.6
1	А	525	ALA	2.5
1	D	341	CYS	2.5
1	D	521	TYR	2.5
1	В	343	VAL	2.5
1	С	527	ASN	2.5
1	А	543	GLU	2.5
1	А	516	ASP	2.4
1	А	466	ILE	2.4
1	В	527	ASN	2.4
1	С	490	ASP	2.4
1	В	463	THR	2.3
1	D	519	SER	2.3
1	А	489	LEU	2.3
1	D	486	LYS	2.3
1	D	579	THR	2.2
1	В	315	TYR	2.1
	<u> </u>		1	



Mol	Chain	Res	Type	RSRZ
1	В	348	ARG	2.1
1	С	532	ILE	2.1
1	А	528	ARG	2.1
1	В	506	ASP	2.1
1	С	570	VAL	2.1
1	D	360	TYR	2.1
1	В	490	ASP	2.1
1	D	347	LEU	2.1
1	В	505	MET	2.1
1	А	546	ALA	2.1
1	D	491	VAL	2.1
1	С	542	PRO	2.0
1	В	360	TYR	2.0
1	В	518	VAL	2.0
1	С	520	PHE	2.0
1	C	568	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	${f B} ext{-factors}({ m \AA}^2)$	Q<0.9
4	CA	D	702	1/1	0.91	0.14	80,80,80,80	0
4	CA	А	702	1/1	0.94	0.19	63,63,63,63	0
3	FE	В	701	1/1	0.95	0.14	42,42,42,42	0
4	CA	В	702	1/1	0.96	0.10	69,69,69,69	0
3	FE	С	701	1/1	0.98	0.18	42,42,42,42	0
3	FE	D	701	1/1	0.99	0.17	35,35,35,35	0
4	CA	С	702	1/1	0.99	0.23	56, 56, 56, 56	0



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q < 0.9
3	FE	А	701	1/1	0.99	0.19	33,33,33,33	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.

