

Full wwPDB X-ray Structure Validation Report (i)

Nov 6, 2023 – 02:31 AM EST

PDB ID	:	6CD1
Title	:	Crystal structure of Medicago truncatula serine hydroxymethyltransferase 3
		(MtSHMT3), complexes with reaction intermediates
Authors	:	Ruszkowski, M.; Sekula, B.; Ruszkowska, A.; Dauter, Z.
Deposited on	:	2018-02-07
Resolution	:	1.91 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	:	1.8.5 (274361), CSD as541be (2020)
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 1.91 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	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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	Δ	455	7%	
1	11	400		•
1	В	455	95% •	•
1	С	455	96%	
		100	7%	_
1	D	455	94%	•
1	F	455	95%	
-	1	100	33.76 •	•



Mol	Chain	Length	Quality of chain	
2	Е	455	96%	
2	G	455	3% 95%	
2	Н	455	94%	5%•

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
6	ACT	С	601	-	-	Х	-



2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 29964 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	459	Total	С	Ν	Ο	\mathbf{S}	0	0	0
1		402	3468	2199	605	649	15	0	0	0
1	В	451	Total	С	Ν	Ο	S	0	3	0
1	D	401	3485	2207	611	652	15	0	5	0
1	С	459	Total	С	Ν	Ο	S	0	1	0
1	U	402	3477	2204	607	651	15	0	1	
1	Л	445	Total	С	Ν	0	S	0	2	0
1		440	3444	2182	604	643	15	0	5	0
1	F	451	Total	С	Ν	Ο	S	0	1	0
	Ľ	401	3466	2195	606	650	15	0	1	U

• Molecule 1 is a protein called Serine hydroxymethyltransferase.

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	79	SER	-	expression tag	UNP G7ILW0
А	80	ASN	-	expression tag	UNP G7ILW0
А	81	ALA	-	expression tag	UNP G7ILW0
В	79	SER	-	expression tag	UNP G7ILW0
В	80	ASN	-	expression tag	UNP G7ILW0
В	81	ALA	-	expression tag	UNP G7ILW0
С	79	SER	-	expression tag	UNP G7ILW0
С	80	ASN	-	expression tag	UNP G7ILW0
С	81	ALA	-	expression tag	UNP G7ILW0
D	79	SER	-	expression tag	UNP G7ILW0
D	80	ASN	-	expression tag	UNP G7ILW0
D	81	ALA	-	expression tag	UNP G7ILW0
F	79	SER	-	expression tag	UNP G7ILW0
F	80	ASN	-	expression tag	UNP G7ILW0
F	81	ALA	-	expression tag	UNP G7ILW0

• Molecule 2 is a protein called Serine hydroxymethyltransferase.



Mol	Chain	Residues		Atoms						AltConf	Trace
2	E	E 451	Total	С	Ν	Ο	Р	\mathbf{S}	0	1	0
2			3481	2203	607	655	1	15	0	I	0
9	C	451	Total	С	Ν	Ο	Р	\mathbf{S}	0	1	0
	G	401	3481	2203	607	655	1	15	0		0
0	ц	452	Total	С	Ν	0	Р	S	0	1	0
		492	3492	2212	608	656	1	15	0		0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Е	79	SER	-	expression tag	UNP G7ILW0
Е	80	ASN	-	expression tag	UNP G7ILW0
E	81	ALA	-	expression tag	UNP G7ILW0
G	79	SER	-	expression tag	UNP G7ILW0
G	80	ASN	-	expression tag	UNP G7ILW0
G	81	ALA	-	expression tag	UNP G7ILW0
Н	79	SER	-	expression tag	UNP G7ILW0
Н	80	ASN	-	expression tag	UNP G7ILW0
Н	81	ALA	-	expression tag	UNP G7ILW0

• Molecule 3 is [3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-YL METHYL]-SERINE (three-letter code: PLS) (formula: C₁₁H₁₇N₂O₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	Λ	1	Total	С	Ν	Ο	Р	0	0
J	A	1	22	11	2	8	1	U	0



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	Л	1	Total	С	Ν	0	Р	0	0
J	D	1	22	11	2	8	1	0	0

• Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	Ε	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	F	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	G	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	Н	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0

• Molecule 5 is N-GLYCINE-[3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-P YRIDIN-4-YL-METHANE] (three-letter code: PLG) (formula: C₁₀H₁₅N₂O₇P) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
5	Р	1	Total	С	Ν	0	Р	0	0
0	D	L	20	10	2	7	1	0	0
5	Б	1	Total	С	Ν	0	Р	0	0
	Г		20	10	2	7	1	0	

• Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
6	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
6	Н	1	Total 4	${ m C} 2$	O 2	0	0

• Molecule 7 is GLYCINE (three-letter code: GLY) (formula: $C_2H_5NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	Е	1	Total 5	$\begin{array}{c} \mathrm{C} \\ \mathrm{2} \end{array}$	N 1	O 2	0	0
7	Н	1	Total 5	С 2	N 1	O 2	0	0

• Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	А	336	Total O 336 336	0	0
8	В	229	Total O 229 229	0	0
8	С	284	Total O 284 284	0	0
8	D	200	Total O 200 200	0	0
8	Е	289	Total O 289 289	0	0
8	F	199	Total O 199 199	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	G	279	Total O 279 279	0	0
8	Н	216	Total O 216 216	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.

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• Molecule 1: Serine hydroxymethyltransferase

• Molecule 1: Serine hydroxymethyltransferase





• Molecule 1: Serine hydroxymethyltransferase

Chain D: 94%







 \bullet Molecule 1: Serine hydroxymethyltransferase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	94.09Å 103.65Å 180.38Å	Depositor
a, b, c, α , β , γ	90.00° 97.38° 90.00°	Depositor
Bosolution(A)	46.65 - 1.91	Depositor
Resolution (A)	46.65 - 1.91	EDS
% Data completeness	98.6 (46.65-1.91)	Depositor
(in resolution range)	$98.7 \ (46.65 - 1.91)$	EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.01 (at 1.91 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
P. P.	0.191 , 0.236	Depositor
n, n_{free}	0.198 , 0.241	DCC
R_{free} test set	1316 reflections (0.50%)	wwPDB-VP
Wilson B-factor $(Å^2)$	35.1	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.32 , 35.3	EDS
L-test for $twinning^2$	$ L > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	29964	wwPDB-VP
Average B, all atoms $(Å^2)$	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 52.82 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.6075e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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: LLP, ACT, EDO, PLS, PLG

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
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.68	0/3540	0.74	0/4788
1	В	0.64	0/3557	0.70	0/4810
1	С	0.63	0/3549	0.70	0/4800
1	D	0.63	0/3513	0.69	0/4747
1	F	0.59	0/3537	0.67	0/4784
2	Ε	0.59	0/3527	0.68	0/4770
2	G	0.62	0/3527	0.68	0/4770
2	Н	0.60	0/3539	0.67	0/4786
All	All	0.62	0/28289	0.69	0/38255

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	3468	0	3467	10	0
1	В	3485	0	3484	11	0
1	С	3477	0	3474	5	0
1	D	3444	0	3441	11	0
1	F	3466	0	3465	6	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Е	3481	0	3469	6	0
2	G	3481	0	3469	4	0
2	Н	3492	0	3478	8	0
3	А	22	0	14	6	0
3	D	22	0	13	4	0
4	А	4	0	6	0	0
4	В	4	0	6	0	0
4	С	4	0	6	1	0
4	D	4	0	6	0	0
4	Е	4	0	6	0	0
4	F	4	0	6	0	0
4	G	4	0	6	0	0
4	Н	4	0	6	0	0
5	В	20	0	12	5	0
5	F	20	0	12	2	0
6	С	8	0	6	2	0
6	Н	4	0	3	0	0
7	Е	5	0	2	0	0
7	Н	5	0	2	1	0
8	А	336	0	0	1	0
8	В	229	0	0	1	0
8	С	284	0	0	2	0
8	D	200	0	0	1	0
8	Е	289	0	0	1	0
8	F	199	0	0	0	0
8	G	279	0	0	0	0
8	Н	216	0	0	0	0
All	All	29964	0	27859	62	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 1.

All (62) 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:A:318:LYS:HZ3	3:A:601:PLS:H4A1	1.52	0.72
1:A:318:LYS:HZ3	3:A:601:PLS:C4A	2.03	0.71
1:F:318:LYS:NZ	5:F:601:PLG:H4A2	2.07	0.69
1:A:318:LYS:NZ	3:A:601:PLS:H4A1	2.09	0.67
1:A:318:LYS:NZ	3:A:601:PLS:C4A	2.59	0.65
1:F:318:LYS:HZ1	5:F:601:PLG:H4A2	1.61	0.65



	A L	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:301:VAL:HG11	1:D:384:VAL:HG21	1.80	0.62
1:D:318[B]:LYS:NZ	3:D:601:PLS:H4A1	2.16	0.61
2:E:468:LYS:H	2:E:468:LYS:CE	2.15	0.59
1:B:318[B]:LYS:HZ1	5:B:601:PLG:H4A2	1.68	0.58
8:C:710:HOH:O	3:D:601:PLS:H4A2	2.06	0.55
2:E:468:LYS:H	2:E:468:LYS:HE3	1.72	0.55
6:C:601:ACT:H2	1:D:134:TYR:OH	2.09	0.53
1:D:257:LYS:NZ	8:D:701:HOH:O	2.41	0.53
1:C:106:PHE:CE2	1:C:526:THR:HG22	2.44	0.53
2:E:482:ARG:NE	8:E:701:HOH:O	2.32	0.53
3:A:601:PLS:H4A2	8:B:706:HOH:O	2.08	0.53
1:D:315:THR:HB	1:D:317[B]:HIS:CE1	2.45	0.52
2:H:198:ARG:HB3	2:H:254:PHE:CE2	2.45	0.51
1:C:144:TYR:HD1	8:C:733:HOH:O	1.95	0.50
6:C:601:ACT:H1	1:D:354:GLY:HA3	1.94	0.49
1:B:503:VAL:HA	1:B:508:PHE:CD1	2.48	0.48
1:A:491:VAL:HG22	1:A:502:PHE:CD2	2.49	0.48
2:E:391:ALA:HB2	2:E:411:VAL:HG11	1.96	0.48
1:A:490:LEU:HD11	8:A:1032:HOH:O	2.15	0.47
1:A:318:LYS:NZ	3:A:601:PLS:N	2.62	0.47
1:D:318[B]:LYS:HZ3	3:D:601:PLS:H4A1	1.79	0.47
1:B:292:HIS:CD2	1:B:318[A]:LYS:HZ3	2.33	0.47
2:H:390:LEU:HD21	2:H:455:ILE:HG21	1.98	0.46
1:D:318[A]:LYS:NZ	3:D:601:PLS:H4A1	2.30	0.46
1:D:317[A]:HIS:O	1:D:318[A]:LYS:HB2	2.15	0.46
1:B:318[A]:LYS:HZ1	5:B:601:PLG:H4A2	1.81	0.45
1:A:518:ARG:O	1:A:522:GLU:HG3	2.15	0.45
1:B:318[B]:LYS:NZ	5:B:601:PLG:H4A2	2.32	0.45
2:H:103:ASP:OD2	2:H:107:ARG:NH2	2.50	0.45
1:F:390:LEU:HD21	1:F:455:ILE:HG21	1.98	0.44
1:B:315:THR:HB	1:B:317[B]:HIS:CE1	2.52	0.44
2:E:390:LEU:HD12	2:E:474:ALA:HB2	2.00	0.44
1:D:292:HIS:O	1:D:319:SER:HB2	2.17	0.44
2:E:387:CYS:SG	2:E:411:VAL:HG13	2.57	0.44
2:H:177:GLN:N	2:H:178:PRO:CD	2.81	0.43
1:F:317:HIS:ND1	1:F:324:ARG:HA	2.33	0.43
2:G:87:LEU:HD21	2:G:98:ILE:HD12	2.00	0.43
1:A:457:SER:N	1:A:458:PRO:CD	2.81	0.43
2:G:391:ALA:HB2	2:G:411:VAL:HG11	2.00	0.43
1:B:223:GLY:HA2	1:B:226:ILE:HD12	2.01	0.43
1:F:182:SER:HB2	1:F:183:PRO:HD3	2.00	0.42



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:158:GLN:HB3	4:C:603:EDO:H12	2.01	0.42
2:G:144:TYR:HH	7:H:602:GLY:N	2.17	0.42
1:B:318[B]:LYS:HZ1	5:B:601:PLG:C4A	2.32	0.42
1:C:112:ILE:HB	1:C:115:GLU:HG3	2.02	0.42
2:H:410:LEU:C	2:H:410:LEU:HD12	2.40	0.41
1:B:409:HIS:CE1	1:B:410:LEU:HD23	2.56	0.41
2:H:114:SER:HB2	2:H:318:LLP:HE3	2.03	0.41
1:A:492:SER:O	2:H:519:ARG:CD	2.69	0.41
2:G:133:LYS:HG2	2:G:150:ILE:HG13	2.02	0.41
1:F:295:GLY:N	1:F:319:SER:OG	2.47	0.41
2:H:390:LEU:HD21	2:H:455:ILE:CG2	2.51	0.41
1:C:87:LEU:HD21	1:C:98:ILE:HD12	2.03	0.40
1:B:410:LEU:HD12	1:B:410:LEU:C	2.42	0.40
1:D:135:SER:CB	1:D:150:ILE:HG21	2.51	0.40
1:B:318[A]:LYS:NZ	5:B:601:PLG:H4A2	2.36	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	Perce	entiles
1	А	450/455~(99%)	439 (98%)	11 (2%)	0	100	100
1	В	452/455~(99%)	437~(97%)	15 (3%)	0	100	100
1	С	451/455~(99%)	440 (98%)	11 (2%)	0	100	100
1	D	442/455~(97%)	424 (96%)	18 (4%)	0	100	100
1	F	450/455~(99%)	442 (98%)	8 (2%)	0	100	100
2	Ε	449/455~(99%)	440 (98%)	9 (2%)	0	100	100
2	G	449/455~(99%)	438 (98%)	11 (2%)	0	100	100
2	Н	450/455~(99%)	440 (98%)	10 (2%)	0	100	100



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percen	tiles
All	All	3593/3640~(99%)	3500~(97%)	93~(3%)	0	100	100

There are no Ramachandran outliers to report.

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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	370/372~(100%)	361~(98%)	9~(2%)	49 41
1	В	372/372~(100%)	362~(97%)	10 (3%)	44 36
1	С	371/372~(100%)	362~(98%)	9~(2%)	49 41
1	D	368/372~(99%)	360~(98%)	8 (2%)	52 45
1	F	370/372~(100%)	361~(98%)	9~(2%)	49 41
2	Ε	369/371~(100%)	364~(99%)	5 (1%)	67 63
2	G	369/371~(100%)	359~(97%)	10 (3%)	44 36
2	Н	370/371~(100%)	359~(97%)	11 (3%)	41 31
All	All	2959/2973~(100%)	2888 (98%)	71 (2%)	49 41

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	134	TYR
1	А	141	LYS
1	А	180	SER
1	А	367	CYS
1	А	390	LEU
1	А	435	THR
1	А	438	LYS
1	А	439	ASN
1	А	482	ARG
1	В	103	ASP
1	В	107	ARG
1	В	134	TYR



Mol	Chain	Res	Type
1	В	180	SER
1	В	218	LYS
1	В	219	ARG
1	В	287	MET
1	В	367	CYS
1	В	439	ASN
1	В	494	THR
1	С	134	TYR
1	С	180	SER
1	С	218	LYS
1	С	219	ARG
1	С	367	CYS
1	С	378	ASN
1	С	412	LEU
1	С	437	ASN
1	С	507	GLU
1	D	134	TYR
1	D	141	LYS
1	D	180	SER
1	D	218	LYS
1	D	219	ARG
1	D	367	CYS
1	D	390	LEU
1	D	445	LYS
2	Е	134	TYR
2	Е	180	SER
2	Е	218	LYS
2	Е	367	CYS
2	Е	468	LYS
1	F	134	TYR
1	F	180	SER
1	F	287	MET
1	F	319	SER
1	F	367	CYS
1	F	403	SER
1	F	439	ASN
1	F	492	SER
1	F	495	LYS
2	G	134	TYR
2	G	141	LYS
2	G	180	SER
2	G	218	LYS



Mol	Chain	Res	Type
2	G	367	CYS
2	G	390	LEU
2	G	436	LEU
2	G	439	ASN
2	G	445	LYS
2	G	494	THR
2	Н	134	TYR
2	Н	141	LYS
2	Н	180	SER
2	Н	218	LYS
2	Н	219	ARG
2	Н	287	MET
2	Н	367	CYS
2	Н	393	ARG
2	Н	411	VAL
2	Н	435	THR
2	Н	504	LEU

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

Mol	Chain	Res	Type
1	В	497	GLN
1	В	501	ASN
1	С	439	ASN
1	D	99	ASN
2	G	99	ASN
2	Н	99	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

3 non-standard protein/DNA/RNA residues 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



Mal	Turne	Chain	Dec Link		Bo	ond leng	ths	B	ond ang	les
1VIOI	туре	Unain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
2	LLP	Е	318	2	23,24,25	1.54	3 (13%)	25,32,34	2.31	9 (36%)
2	LLP	Н	318	2	23,24,25	1.72	5 (21%)	25,32,34	2.30	8 (32%)
2	LLP	G	318	2	23,24,25	1.52	5 (21%)	25,32,34	1.97	7 (28%)

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).

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	LLP	Е	318	2	-	10/16/17/19	0/1/1/1
2	LLP	Н	318	2	-	5/16/17/19	0/1/1/1
2	LLP	G	318	2	-	6/16/17/19	0/1/1/1

All	(13)	bond	length	outliers	are	listed	below:
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Mol	Chain	Res	Type	Atoms	Z	$Observed(\text{\AA})$	Ideal(Å)
2	Е	318	LLP	C4-C4'	4.25	1.54	1.46
2	Н	318	LLP	C4-C5	-4.18	1.36	1.42
2	G	318	LLP	C4-C4'	3.97	1.54	1.46
2	Н	318	LLP	C4-C4'	3.67	1.53	1.46
2	Н	318	LLP	C3-C2	-3.10	1.37	1.40
2	Н	318	LLP	CB-CA	2.75	1.57	1.53
2	G	318	LLP	CB-CA	2.48	1.56	1.53
2	Ε	318	LLP	C4-C5	-2.48	1.38	1.42
2	G	318	LLP	C2'-C2	2.37	1.54	1.50
2	Е	318	LLP	CB-CA	2.32	1.56	1.53
2	Н	318	LLP	C4-C3	-2.08	1.37	1.40
2	G	318	LLP	P-OP4	2.06	1.66	1.60
2	G	318	LLP	C4-C3	-2.05	1.37	1.40

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^{o})$	$Ideal(^{o})$
2	Е	318	LLP	CE-NZ-C4'	6.95	140.23	118.90
2	Н	318	LLP	OP4-C5'-C5	6.21	121.17	109.35
2	Н	318	LLP	CE-NZ-C4'	5.57	136.02	118.90
2	G	318	LLP	CE-NZ-C4'	4.98	134.21	118.90



Mol	Chain	\mathbf{Res}	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
2	G	318	LLP	OP4-C5'-C5	4.34	117.62	109.35
2	Е	318	LLP	C5'-C5-C6	-4.01	112.78	119.37
2	Е	318	LLP	C4-C4'-NZ	-3.56	107.94	124.31
2	Н	318	LLP	C4-C4'-NZ	-3.27	109.28	124.31
2	G	318	LLP	C4-C4'-NZ	-3.13	109.94	124.31
2	Е	318	LLP	C5-C4-C4'	3.06	126.59	121.56
2	Н	318	LLP	C3-C4-C5	2.99	120.56	118.26
2	Е	318	LLP	OP4-C5'-C5	2.93	114.93	109.35
2	Н	318	LLP	OP3-P-OP4	2.90	114.45	106.73
2	Н	318	LLP	C3-C2-N1	-2.75	117.22	120.77
2	G	318	LLP	C5-C6-N1	-2.70	119.33	123.82
2	Е	318	LLP	C3-C4-C4'	-2.68	115.43	120.41
2	G	318	LLP	C5'-C5-C6	-2.52	115.22	119.37
2	G	318	LLP	OP2-P-OP4	2.38	113.06	106.73
2	Е	318	LLP	C4-C3-C2	2.32	121.62	120.19
2	Н	318	LLP	C5-C6-N1	-2.29	120.00	123.82
2	Е	318	LLP	C5-C6-N1	-2.22	120.12	123.82
2	Н	318	LLP	C4-C3-C2	2.18	121.54	120.19
2	G	318	LLP	C3-C4-C4'	-2.12	116.46	120.41
2	Е	318	LLP	C2'-C2-C3	2.02	123.39	120.89

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms
2	Е	318	LLP	C5-C4-C4'-NZ
2	Е	318	LLP	C6-C5-C5'-OP4
2	Е	318	LLP	C5'-OP4-P-OP3
2	Е	318	LLP	O-C-CA-CB
2	Е	318	LLP	CG-CD-CE-NZ
2	G	318	LLP	O-C-CA-CB
2	Н	318	LLP	O-C-CA-CB
2	Н	318	LLP	CG-CD-CE-NZ
2	G	318	LLP	CG-CD-CE-NZ
2	G	318	LLP	C3-C4-C4'-NZ
2	Н	318	LLP	C5-C4-C4'-NZ
2	Н	318	LLP	C3-C4-C4'-NZ
2	Е	318	LLP	C3-C4-C4'-NZ
2	G	318	LLP	C5-C4-C4'-NZ
2	Е	318	LLP	C5'-OP4-P-OP2
2	G	318	LLP	CD-CE-NZ-C4'
2	Е	318	LLP	C4-C5-C5'-OP4



Mol	Chain	Res	Type	Atoms
2	Е	318	LLP	CD-CE-NZ-C4'
2	Н	318	LLP	CD-CE-NZ-C4'
2	Ε	318	LLP	C5'-OP4-P-OP1
2	G	318	LLP	N-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Н	318	LLP	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

17 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).

Mal	Turne	Chain	Dec	Tink	Bo	ond leng	ths	Bond angles		
IVIOI	туре	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
4	EDO	С	603	-	3,3,3	0.32	0	2,2,2	0.36	0
6	ACT	Н	601	-	3,3,3	0.89	0	3,3,3	0.77	0
6	ACT	С	602	-	3,3,3	0.88	0	$3,\!3,\!3$	1.37	0
7	GLY	Е	601	-	4,4,4	1.09	1 (25%)	$3,\!4,\!4$	2.46	2 (66%)
5	PLG	В	601	-	20,20,20	1.57	2 (10%)	$25,\!28,\!28$	2.80	7 (28%)
3	PLS	А	601	-	22,22,22	2.01	3 (13%)	27,31,31	1.99	6 (22%)
4	EDO	F	602	-	3,3,3	0.46	0	2,2,2	0.37	0
4	EDO	G	601	-	3,3,3	0.47	0	2,2,2	0.33	0
4	EDO	А	602	-	3,3,3	0.51	0	2,2,2	0.22	0
6	ACT	С	601	-	3,3,3	0.53	0	3,3,3	1.35	0
3	PLS	D	601	-	22,22,22	1.74	3 (13%)	27,31,31	2.15	6 (22%)



Mal	Turne	Chain	Dec	Tiple	Bo	ond leng	$_{\rm ths}$	Bond angles		
WIOI	туре	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
5	PLG	F	601	-	20,20,20	1.49	4 (20%)	25,28,28	2.78	7 (28%)
4	EDO	Н	603	-	3,3,3	0.44	0	2,2,2	0.41	0
4	EDO	D	602	-	3,3,3	0.44	0	2,2,2	0.47	0
7	GLY	Н	602	-	4,4,4	1.24	1 (25%)	3,4,4	2.27	2 (66%)
4	EDO	В	602	-	3,3,3	0.48	0	2,2,2	0.19	0
4	EDO	E	602	-	3,3,3	0.52	0	2,2,2	0.29	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
4	EDO	С	603	-	-	0/1/1/1	-
7	GLY	Е	601	-	-	0/2/2/2	-
5	PLG	В	601	-	-	4/12/12/12	0/1/1/1
3	PLS	А	601	-	-	7/17/17/17	0/1/1/1
4	EDO	F	602	-	-	0/1/1/1	-
4	EDO	G	601	-	-	0/1/1/1	-
4	EDO	А	602	-	-	1/1/1/1	-
3	PLS	D	601	-	-	5/17/17/17	0/1/1/1
5	PLG	F	601	-	-	3/12/12/12	0/1/1/1
4	EDO	Н	603	-	-	0/1/1/1	-
4	EDO	D	602	-	-	0/1/1/1	-
7	GLY	Н	602	-	-	0/2/2/2	-
4	EDO	В	602	-	-	0/1/1/1	-
4	EDO	Ē	602	-	-	0/1/1/1	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
3	А	601	PLS	C4A-N	-6.66	1.27	1.46
3	D	601	PLS	C4A-N	-6.11	1.28	1.46
5	В	601	PLG	C4A-N	-4.05	1.27	1.46
5	F	601	PLG	C4A-N	-3.92	1.27	1.46
3	А	601	PLS	C3-C2	-3.54	1.37	1.40
3	А	601	PLS	C2A-C2	2.90	1.55	1.50
5	F	601	PLG	C4A-C4	2.45	1.55	1.51
7	Н	602	GLY	OXT-C	-2.43	1.22	1.30
5	В	601	PLG	C2A-C2	2.37	1.54	1.50
3	D	601	PLS	P-O4P	2.18	1.67	1.60



Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
5	F	601	PLG	P-OP4	2.15	1.67	1.60
3	D	601	PLS	C4A-C4	2.15	1.54	1.51
7	Е	601	GLY	OXT-C	-2.14	1.23	1.30
5	F	601	PLG	C2A-C2	2.02	1.53	1.50

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	В	601	PLG	C4A-N-CA	10.88	123.94	112.58
5	F	601	PLG	C4A-N-CA	10.64	123.68	112.58
3	D	601	PLS	C4A-N-CA	9.07	131.11	113.92
3	А	601	PLS	C4A-N-CA	5.95	125.19	113.92
5	F	601	PLG	C4-C4A-N	5.35	121.57	111.58
5	В	601	PLG	C4-C4A-N	4.97	120.86	111.58
3	А	601	PLS	O4P-C5A-C5	4.15	117.27	109.35
7	Н	602	GLY	OXT-C-O	-3.24	115.22	123.30
5	F	601	PLG	OP4-C5A-C5	3.08	115.22	109.35
3	А	601	PLS	C5-C6-N1	-3.07	118.70	123.82
7	Е	601	GLY	OXT-C-O	-3.02	115.77	123.30
5	В	601	PLG	C5-C6-N1	-3.00	118.82	123.82
3	А	601	PLS	C4-C4A-N	2.96	119.94	111.78
7	Е	601	GLY	OXT-C-CA	2.91	125.03	113.45
5	F	601	PLG	OXT-C-CA	2.79	122.42	112.74
3	А	601	PLS	C6-N1-C2	2.77	124.29	119.17
3	D	601	PLS	C6-C5-C4	2.66	120.00	118.12
5	F	601	PLG	C5-C6-N1	-2.52	119.62	123.82
3	D	601	PLS	OXT-C-O	-2.48	118.46	124.09
5	F	601	PLG	C5A-C5-C6	-2.47	115.30	119.37
3	D	601	PLS	C5-C6-N1	-2.44	119.75	123.82
3	D	601	PLS	OXT-C-CA	2.39	121.36	113.40
5	В	601	PLG	OP4-P-OP1	2.29	112.91	106.47
5	F	601	PLG	C6-C5-C4	2.27	119.72	118.12
3	А	601	PLS	C5A-C5-C6	-2.27	115.64	119.37
7	Н	602	GLY	OXT-C-CA	2.24	122.36	113.45
3	D	601	PLS	C4-C4A-N	2.22	117.89	111.78
5	В	601	PLG	OP4-C5A-C5	2.19	113.52	109.35
5	В	601	PLG	C6-N1-C2	2.17	123.19	119.17
5	В	601	PLG	OXT-C-CA	2.15	120.19	112.74

There are no chirality outliers.

All (20) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
3	А	601	PLS	C-CA-N-C4A
3	А	601	PLS	C-CA-CB-OG
3	А	601	PLS	C3-C4-C4A-N
3	А	601	PLS	C5-C4-C4A-N
3	D	601	PLS	C5-C4-C4A-N
5	В	601	PLG	C5-C4-C4A-N
5	F	601	PLG	C5-C4-C4A-N
3	А	601	PLS	N-CA-CB-OG
5	F	601	PLG	C3-C4-C4A-N
3	D	601	PLS	C-CA-N-C4A
3	D	601	PLS	C3-C4-C4A-N
5	В	601	PLG	C3-C4-C4A-N
3	А	601	PLS	CB-CA-N-C4A
3	D	601	PLS	CB-CA-N-C4A
5	В	601	PLG	C-CA-N-C4A
5	F	601	PLG	C-CA-N-C4A
3	A	601	PLS	C5A-O4P-P-O3P
5	В	601	PLG	C5A-OP4-P-OP3
4	А	602	EDO	O1-C1-C2-O2
3	D	601	PLS	C-CA-CB-OG

There are no ring outliers.

7 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	С	603	EDO	1	0
5	В	601	PLG	5	0
3	А	601	PLS	6	0
6	С	601	ACT	2	0
3	D	601	PLS	4	0
5	F	601	PLG	2	0
7	Н	602	GLY	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	$\langle RSRZ \rangle$	#RSRZ	i>2	$OWAB(Å^2)$	Q < 0.9
1	А	452/455~(99%)	0.25	34 (7%) 14	16	21, 32, 56, 78	0
1	В	451/455~(99%)	0.27	28 (6%) 20	23	22, 38, 58, 84	0
1	С	452/455~(99%)	0.21	17 (3%) 40	43	28, 38, 58, 76	0
1	D	445/455~(97%)	0.35	30 (6%) 17	20	28, 41, 76, 98	0
1	F	451/455~(99%)	0.30	23 (5%) 28	31	28, 43, 63, 82	0
2	Ε	450/455~(98%)	0.13	18 (4%) 38	41	26, 36, 58, 83	0
2	G	450/455~(98%)	0.13	13 (2%) 51	55	28, 39, 54, 81	0
2	Н	451/455~(99%)	0.35	24 (5%) 26	29	27, 43, 62, 89	0
All	All	3602/3640~(98%)	0.25	187 (5%) 2	7 30	21, 39, 61, 98	0

All (187) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Н	506	PRO	8.2
1	D	504	LEU	6.0
1	D	500	LEU	5.2
1	А	506	PRO	5.0
2	Н	390	LEU	4.7
1	D	395	VAL	4.7
1	А	82	PHE	4.7
1	В	506	PRO	4.6
1	А	492	SER	4.2
1	F	445	LYS	4.1
2	Е	143	TYR	4.0
2	Н	82	PHE	4.0
1	А	179	LEU	4.0
2	Н	468	LYS	3.9
1	D	378	ASN	3.8
2	G	179	LEU	3.8



Mol	Chain	Res	Type	RSRZ
2	Е	179	LEU	3.8
1	D	179	LEU	3.8
1	F	179	LEU	3.7
1	D	464	GLY	3.6
1	D	503	VAL	3.6
2	Е	83	LEU	3.6
1	В	179	LEU	3.6
2	Н	465	LEU	3.6
2	Е	492	SER	3.6
1	В	492	SER	3.5
2	Н	83	LEU	3.5
1	В	217	ALA	3.4
2	Н	378	ASN	3.3
1	D	384	VAL	3.3
2	G	468	LYS	3.3
2	Е	144	TYR	3.3
2	G	529	PRO	3.2
1	А	348	VAL	3.2
2	Н	472	LEU	3.2
2	Н	507	GLU	3.2
1	С	278	ILE	3.2
1	D	528	TYR	3.1
1	С	205	PRO	3.1
1	А	487	ALA	3.1
1	В	505	ALA	3.1
2	Н	143	TYR	3.1
1	А	178	PRO	3.0
1	D	139	PRO	3.0
1	F	468	LYS	3.0
1	В	178	PRO	3.0
1	В	448	LEU	2.9
1	F	472	LEU	2.9
1	D	508	PHE	2.9
2	Н	494	THR	2.9
1	D	143	TYR	2.9
1	A	176	VAL	2.9
1	А	360	THR	2.9
1	А	328	ILE	2.9
1	А	326	GLY	2.9
2	G	253	LEU	2.8
1	А	184	ALA	2.8
1	В	445	LYS	2.8



Mol	Chain	Res	Type	RSRZ
1	А	143	TYR	2.8
1	D	389	ALA	2.8
2	Н	389	ALA	2.8
1	D	489	SER	2.8
2	Н	302	LEU	2.8
1	D	374	PRO	2.8
1	С	468	LYS	2.8
2	Н	387	CYS	2.8
1	А	354	GLY	2.7
1	В	184	ALA	2.7
1	D	527	GLN	2.7
1	D	490	LEU	2.7
1	В	176	VAL	2.7
1	В	361	ILE	2.7
1	В	218	LYS	2.7
1	D	521	VAL	2.7
1	В	507	GLU	2.6
1	D	109	LEU	2.6
1	А	504	LEU	2.6
1	D	516	ASN	2.6
2	Н	279	ALA	2.6
1	F	83	LEU	2.6
1	В	348	VAL	2.6
1	С	130	LEU	2.5
1	F	184	ALA	2.5
1	F	496	VAL	2.5
1	F	505	ALA	2.5
1	В	183	PRO	2.5
1	С	83	LEU	2.5
2	Е	493	GLY	2.5
1	D	388	ARG	2.4
1	А	180	SER	2.4
1	С	184	ALA	2.4
1	А	491	VAL	2.4
1	С	470	PHE	2.4
2	G	183	PRO	2.4
2	Н	85	TYR	2.4
1	В	354	GLY	2.4
2	G	348	VAL	2.4
1	В	326	GLY	2.4
1	А	501	ASN	2.4
2	Е	348	VAL	2.4



Mol	Chain	Res	Type	RSRZ
1	С	472	LEU	2.4
1	В	180	SER	2.4
1	В	494	THR	2.4
1	D	352	LEU	2.3
1	F	217	ALA	2.3
2	G	218	LYS	2.3
2	Н	523	ALA	2.3
1	D	502	PHE	2.3
1	А	315	THR	2.3
1	F	325	GLY	2.3
1	С	348	VAL	2.3
1	А	490	LEU	2.3
2	Е	184	ALA	2.3
2	Е	364	LEU	2.3
2	Е	326	GLY	2.3
2	G	506	PRO	2.3
2	Е	182	SER	2.3
1	А	359	HIS	2.3
1	F	348	VAL	2.3
1	А	505	ALA	2.3
1	F	412	LEU	2.3
1	F	219	ARG	2.3
2	Е	491	VAL	2.3
2	Е	320	LEU	2.3
1	F	360	THR	2.2
1	F	506	PRO	2.2
2	G	246	MET	2.2
2	Е	494	THR	2.2
2	Н	303	ALA	2.2
2	Е	361	ILE	2.2
1	F	218	LYS	2.2
1	А	508	PHE	2.2
2	Н	348	VAL	2.2
1	А	182	SER	2.2
1	А	316	THR	2.2
1	D	520	LYS	2.2
1	В	125	ALA	2.2
2	Н	184	ALA	2.2
1	С	270	ILE	2.2
1	F	178	PRO	2.2
2	G	249	LYS	2.2
1	В	352	LEU	2.2



GCI	D1
	$\mathcal{D}1$

Mol	Chain	Res	Type	RSRZ	
2	G	83	LEU	2.2	
1	А	187	ALA	2.2	
1	С	507	GLU	2.2	
2	G	378	ASN	2.2	
1	В	186	PHE	2.2	
1	В	83	LEU	2.1	
1	В	316	THR	2.1	
1	В	320	LEU	2.1	
1	F	524	LEU	2.1	
2	Н	301	VAL	2.1	
1	С	216	THR	2.1	
2	Е	140	GLY	2.1	
1	В	347	ALA	2.1	
1	С	502	PHE	2.1	
1	D	445	LYS	2.1	
2	Н	470	PHE	2.1	
1	В	325	GLY	2.1	
1	А	500	LEU	2.1	
2	Е	145	GLY	2.1	
1	F	470	PHE	2.1	
1	F	176	VAL	2.1	
1	А	320	LEU	2.1	
1	С	247	LEU	2.1	
1	F	448	LEU	2.1	
2	G	504	LEU	2.1	
1	С	170	ASP	2.1	
2	Н	178	PRO	2.1	
1	С	144	TYR	2.1	
1	D	85	TYR	2.1	
1	D	134	TYR	2.1	
1	В	314	THR	2.1	
1	А	186	PHE	2.1	
1	А	447	ALA	2.1	
1	F	183	PRO	2.1	
2	Е	130	LEU	2.1	
1	А	325	GLY	2.1	
2	Н	370	TYR	2.0	
1	F	180	SER	2.0	
1	А	366	VAL	2.0	
1	D	468	LYS	2.0	
1	А	507	GLU	2.0	
1	D	482	ARG	2.0	



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Mol	Chain	Res	Type	RSRZ
1	D	385	ALA	2.0
1	А	364	LEU	2.0
1	С	361	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	LLP	G	318	24/25	0.92	0.16	$39,\!48,\!53,\!54$	0
2	LLP	Н	318	24/25	0.94	0.12	32,38,42,45	0
2	LLP	Е	318	24/25	0.96	0.12	30,34,39,40	0

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
6	ACT	Н	601	4/4	0.84	0.26	$55,\!56,\!58,\!59$	0
6	ACT	С	602	4/4	0.87	0.37	$57,\!59,\!60,\!63$	0
4	EDO	Е	602	4/4	0.87	0.13	$49,\!53,\!54,\!57$	0
7	GLY	Н	602	5/5	0.91	0.20	49,49,50,51	0
5	PLG	F	601	20/20	0.92	0.13	$40,\!49,\!56,\!57$	0
7	GLY	Е	601	5/5	0.92	0.13	45,45,47,48	0
4	EDO	D	602	4/4	0.92	0.12	$55,\!55,\!56,\!56$	0
4	EDO	F	602	4/4	0.93	0.10	43,46,47,49	0
6	ACT	С	601	4/4	0.94	0.26	36, 36, 37, 38	0
3	PLS	D	601	22/22	0.94	0.12	32,38,50,56	0
4	EDO	Н	603	4/4	0.94	0.10	48,50,51,53	0
5	PLG	В	601	20/20	0.94	0.13	36,40,48,48	0



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}(\operatorname{\AA}^2)$	Q<0.9
4	EDO	В	602	4/4	0.94	0.14	$35,\!38,\!39,\!40$	0
4	EDO	С	603	4/4	0.95	0.11	42,42,43,43	0
4	EDO	А	602	4/4	0.95	0.11	41,43,44,46	0
3	PLS	А	601	22/22	0.95	0.13	27,29,37,43	0
4	EDO	G	601	4/4	0.98	0.07	39,42,42,44	0

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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.

