



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:16 PM GMT

PDB ID : 4KYI
Title : Crystal structure of the phospholipase VipD from Legionella pneumophila in complex with the human GTPase Rab5
Authors : Lucas, M.; Gaspar, A.H.; Pallara, C.; Rojas, A.L.; Fernandez-Recio, J.; Machner, M.P.; Hierro, A.
Deposited on : 2013-05-29
Resolution : 3.08 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

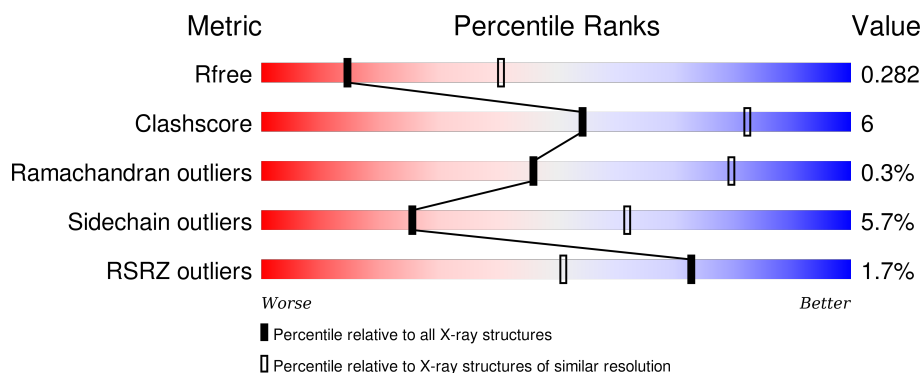
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.08 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}	91344	1119 (3.12-3.04)
Clashscore	102246	1098 (3.10-3.06)
Ramachandran outliers	100387	1057 (3.10-3.06)
Sidechain outliers	100360	1057 (3.10-3.06)
RSRZ outliers	91569	1001 (3.10-3.06)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$. 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	551	<div> <div></div> <div>78%17% . .</div> </div>
1	C	551	<div> <div>3%</div> <div>74%20% . .</div> </div>
1	E	551	<div> <div></div> <div>75%19% . .</div> </div>
1	G	551	<div> <div>4%</div> <div>75%19% . .</div> </div>
2	B	170	<div> <div></div> <div>80%16% .</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	170	 79% 16% • •
2	F	170	 85% 11% •
2	H	170	 84% 12% • •

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
3	EDO	B	302	-	-	-	X
3	EDO	B	303	-	-	-	X
4	GOL	A	604	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 21833 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called VipD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	530	Total	C	N	O	S	0	0	0
			4140	2608	708	807	17			
1	C	527	Total	C	N	O	S	0	0	0
			4120	2596	705	802	17			
1	E	531	Total	C	N	O	S	0	0	0
			4145	2609	709	810	17			
1	G	528	Total	C	N	O	S	0	0	0
			4122	2594	705	806	17			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	GLY	-	EXPRESSION TAG	UNP Q5ZRP9
A	15	ALA	-	EXPRESSION TAG	UNP Q5ZRP9
A	16	MET	-	EXPRESSION TAG	UNP Q5ZRP9
A	17	GLY	-	EXPRESSION TAG	UNP Q5ZRP9
A	18	SER	-	EXPRESSION TAG	UNP Q5ZRP9
C	14	GLY	-	EXPRESSION TAG	UNP Q5ZRP9
C	15	ALA	-	EXPRESSION TAG	UNP Q5ZRP9
C	16	MET	-	EXPRESSION TAG	UNP Q5ZRP9
C	17	GLY	-	EXPRESSION TAG	UNP Q5ZRP9
C	18	SER	-	EXPRESSION TAG	UNP Q5ZRP9
E	14	GLY	-	EXPRESSION TAG	UNP Q5ZRP9
E	15	ALA	-	EXPRESSION TAG	UNP Q5ZRP9
E	16	MET	-	EXPRESSION TAG	UNP Q5ZRP9
E	17	GLY	-	EXPRESSION TAG	UNP Q5ZRP9
E	18	SER	-	EXPRESSION TAG	UNP Q5ZRP9
G	14	GLY	-	EXPRESSION TAG	UNP Q5ZRP9
G	15	ALA	-	EXPRESSION TAG	UNP Q5ZRP9
G	16	MET	-	EXPRESSION TAG	UNP Q5ZRP9
G	17	GLY	-	EXPRESSION TAG	UNP Q5ZRP9
G	18	SER	-	EXPRESSION TAG	UNP Q5ZRP9

- Molecule 2 is a protein called Ras-related protein Rab-5C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	164	Total	C	N	O	S	0	0	0
			1283	820	215	242	6			
2	D	164	Total	C	N	O	S	0	0	0
			1283	820	215	242	6			
2	F	164	Total	C	N	O	S	0	0	0
			1283	820	215	242	6			
2	H	164	Total	C	N	O	S	0	0	0
			1283	820	215	242	6			

There are 24 discrepancies between the modelled and reference sequences:

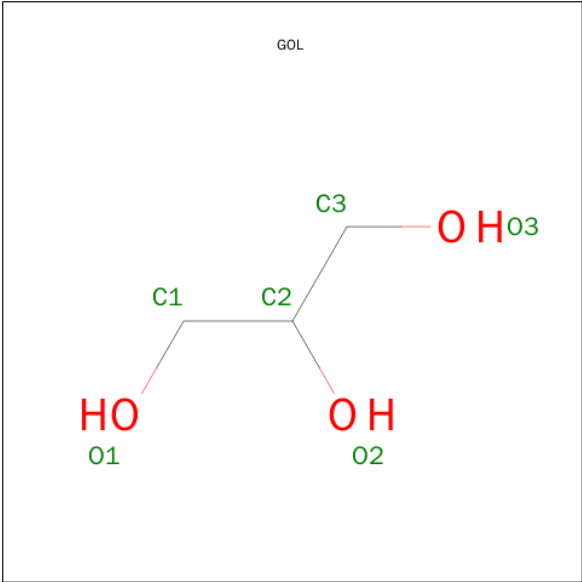
Chain	Residue	Modelled	Actual	Comment	Reference
B	13	GLY	-	EXPRESSION TAG	UNP P51148
B	14	ALA	-	EXPRESSION TAG	UNP P51148
B	15	MET	-	EXPRESSION TAG	UNP P51148
B	16	GLY	-	EXPRESSION TAG	UNP P51148
B	17	SER	-	EXPRESSION TAG	UNP P51148
B	80	LEU	GLN	ENGINEERED MUTATION	UNP P51148
D	13	GLY	-	EXPRESSION TAG	UNP P51148
D	14	ALA	-	EXPRESSION TAG	UNP P51148
D	15	MET	-	EXPRESSION TAG	UNP P51148
D	16	GLY	-	EXPRESSION TAG	UNP P51148
D	17	SER	-	EXPRESSION TAG	UNP P51148
D	80	LEU	GLN	ENGINEERED MUTATION	UNP P51148
F	13	GLY	-	EXPRESSION TAG	UNP P51148
F	14	ALA	-	EXPRESSION TAG	UNP P51148
F	15	MET	-	EXPRESSION TAG	UNP P51148
F	16	GLY	-	EXPRESSION TAG	UNP P51148
F	17	SER	-	EXPRESSION TAG	UNP P51148
F	80	LEU	GLN	ENGINEERED MUTATION	UNP P51148
H	13	GLY	-	EXPRESSION TAG	UNP P51148
H	14	ALA	-	EXPRESSION TAG	UNP P51148
H	15	MET	-	EXPRESSION TAG	UNP P51148
H	16	GLY	-	EXPRESSION TAG	UNP P51148
H	17	SER	-	EXPRESSION TAG	UNP P51148
H	80	LEU	GLN	ENGINEERED MUTATION	UNP P51148

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



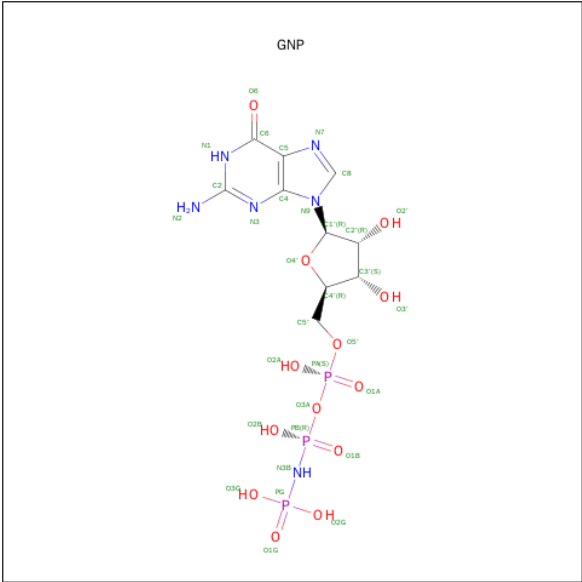
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	G	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
5	D	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
5	F	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
5	H	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

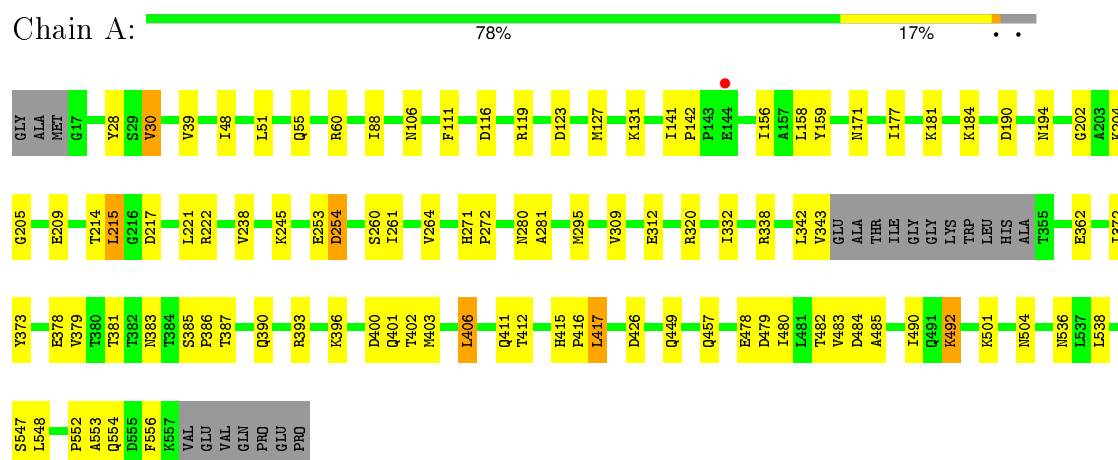
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	1	Total	Mg	0	0
			1	1		
6	B	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		
6	F	1	Total	Mg	0	0
			1	1		

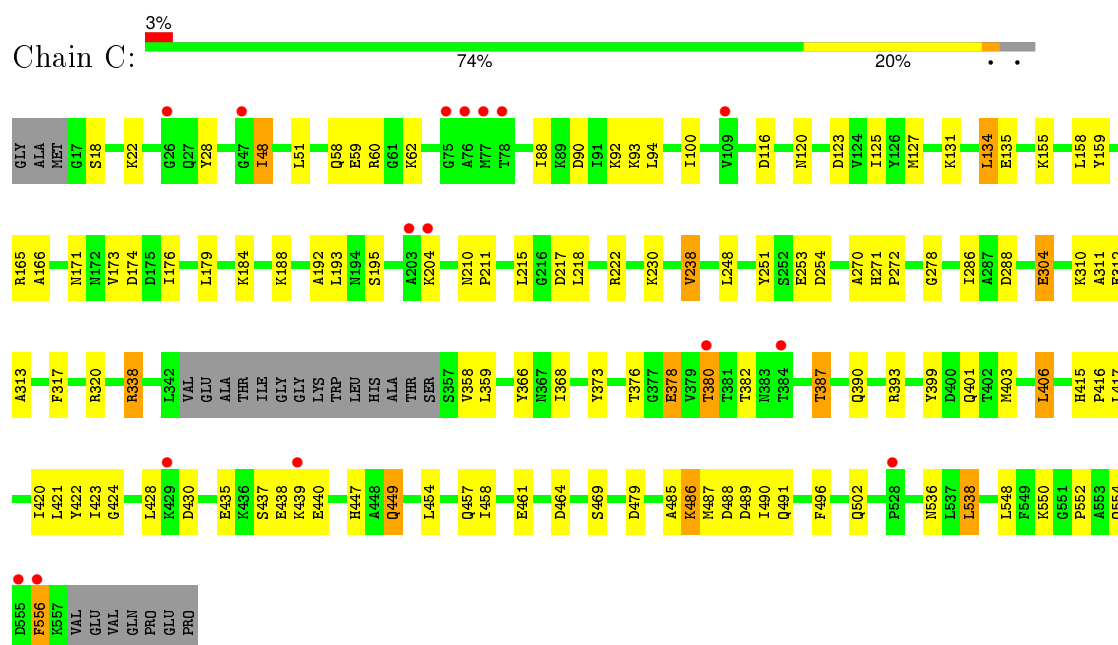
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: VipD

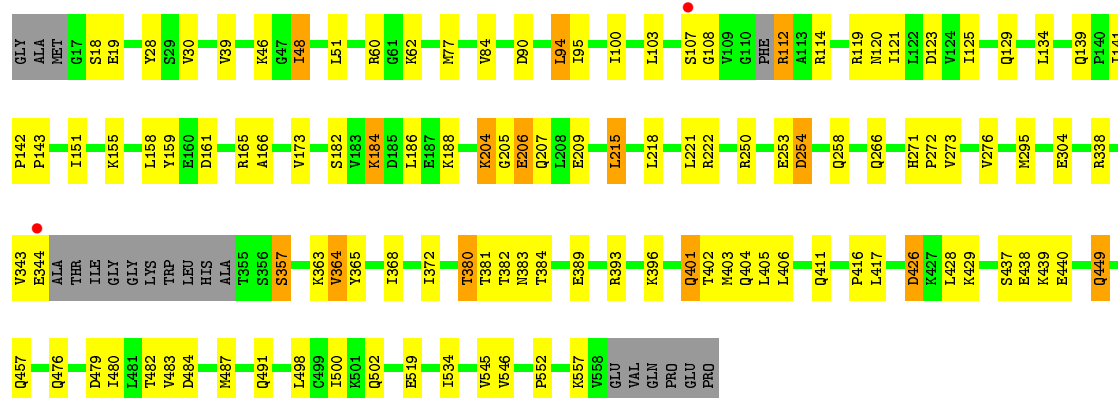


• Molecule 1: VipD




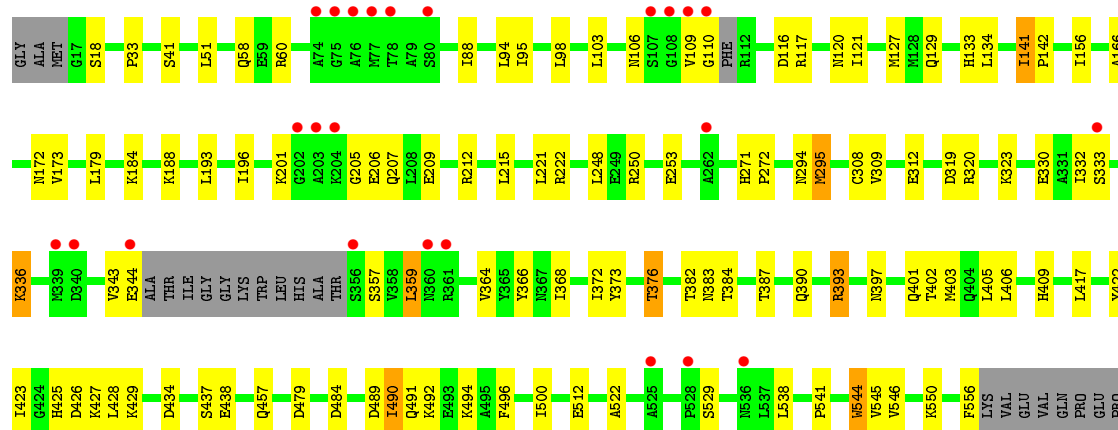
• Molecule 1: VipD

Chain E: 




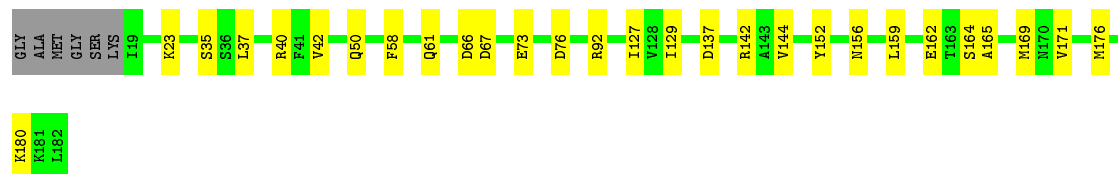
• Molecule 1: VipD

Chain G: 




• Molecule 2: Ras-related protein Rab-5C

Chain B: 



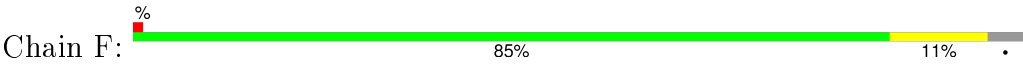
• Molecule 2: Ras-related protein Rab-5C

Chain D: 

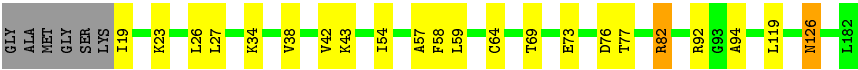
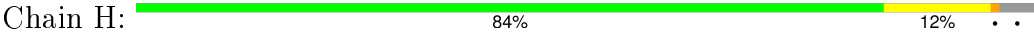




• Molecule 2: Ras-related protein Rab-5C



• Molecule 2: Ras-related protein Rab-5C



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	94.28Å 97.98Å 109.85Å 76.57° 80.71° 78.91°	Depositor
Resolution (Å)	29.83 – 3.08 29.83 – 3.07	Depositor EDS
% Data completeness (in resolution range)	97.6 (29.83-3.08) 91.7 (29.83-3.07)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 3.06Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.233 , 0.280 0.232 , 0.282	Depositor DCC
R_{free} test set	3407 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	85.7	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 27.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 67490 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	21833	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, GNP, MG, EDO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.22	0/4202	0.39	0/5668
1	C	0.22	0/4182	0.38	0/5640
1	E	0.22	0/4205	0.39	0/5671
1	G	0.21	0/4182	0.38	0/5640
2	B	0.23	0/1305	0.39	0/1765
2	D	0.22	0/1305	0.38	0/1765
2	F	0.22	0/1305	0.37	0/1765
2	H	0.23	0/1305	0.39	0/1765
All	All	0.22	0/21991	0.38	0/29679

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4140	0	4187	45	0
1	C	4120	0	4166	65	0
1	E	4145	0	4192	61	0
1	G	4122	0	4163	58	0
2	B	1283	0	1282	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1283	0	1282	21	0
2	F	1283	0	1282	15	0
2	H	1283	0	1282	15	0
3	A	8	0	12	1	0
3	B	8	0	12	1	0
3	E	4	0	6	0	0
3	G	4	0	6	2	0
4	A	12	0	16	0	0
4	E	6	0	8	1	0
5	B	32	0	13	0	0
5	D	32	0	13	4	0
5	F	32	0	13	1	0
5	H	32	0	13	1	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
6	H	1	0	0	0	0
All	All	21833	0	21948	279	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 (279) 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:E:112:ARG:HD3	1:E:276:VAL:HG12	1.68	0.75
1:C:312:GLU:OE2	1:C:320:ARG:NH1	2.22	0.72
1:C:58:GLN:HG2	1:C:88:ILE:HD12	1.72	0.72
1:E:112:ARG:NH2	1:E:272:PRO:O	2.27	0.68
1:E:60:ARG:HG3	1:E:406:LEU:HD23	1.74	0.68
1:G:457:GLN:HG3	2:H:58:PHE:HE1	1.58	0.68
1:C:338:ARG:NH2	1:C:536:ASN:OD1	2.27	0.68
1:C:60:ARG:HG3	1:C:406:LEU:HD23	1.77	0.66
1:G:312:GLU:OE2	1:G:320:ARG:NH1	2.29	0.66
1:E:222:ARG:NH2	1:E:253:GLU:OE2	2.29	0.65
1:E:19:GLU:HG2	1:E:429:LYS:HG2	1.78	0.65
2:H:23:LYS:HA	2:H:73:GLU:HB2	1.78	0.64
1:E:479:ASP:OD2	2:F:92:ARG:NH1	2.30	0.64
1:C:359:LEU:HD13	1:C:538:LEU:HD22	1.80	0.64
1:E:90:ASP:HB3	1:E:173:VAL:HG21	1.80	0.63
1:E:28:TYR:OH	1:E:440:GLU:OE2	2.16	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:215:LEU:HB3	1:E:253:GLU:HA	1.81	0.62
1:G:215:LEU:HB3	1:G:253:GLU:HA	1.82	0.62
1:A:457:GLN:HG3	2:B:58:PHE:HE1	1.64	0.62
1:E:487:MET:HB3	1:E:491:GLN:HG3	1.82	0.62
1:C:437:SER:HB3	1:C:438:GLU:HB2	1.82	0.62
1:E:30:VAL:HG21	1:E:411:GLN:HE21	1.64	0.62
1:C:222:ARG:NH2	1:C:253:GLU:OE2	2.31	0.62
1:E:119:ARG:NH1	1:E:120:ASN:OD1	2.32	0.62
1:E:46:LYS:NZ	1:E:380:THR:O	2.33	0.62
1:G:103:LEU:HD22	1:G:121:ILE:HG13	1.82	0.62
1:G:250:ARG:NH1	3:G:601:EDO:O1	2.32	0.62
1:E:254:ASP:N	1:E:254:ASP:OD1	2.33	0.61
1:A:396:LYS:NZ	1:A:400:ASP:OD2	2.31	0.61
2:F:42:VAL:HG22	2:F:61:GLN:HB2	1.82	0.61
1:E:107:SER:OG	1:E:114:ARG:NH1	2.34	0.61
1:C:28:TYR:OH	1:C:440:GLU:OE2	2.12	0.61
1:A:60:ARG:HD2	1:A:406:LEU:HD23	1.83	0.60
1:E:161:ASP:OD1	1:E:165:ARG:NH1	2.34	0.59
2:B:142:ARG:NH1	2:B:144:VAL:O	2.35	0.59
1:A:479:ASP:OD2	2:B:92:ARG:NH1	2.35	0.59
1:A:484:ASP:OD2	2:B:92:ARG:NH2	2.35	0.59
1:C:116:ASP:O	1:C:120:ASN:ND2	2.36	0.59
1:C:487:MET:HB3	1:C:491:GLN:HG3	1.85	0.59
1:A:338:ARG:NH2	1:A:536:ASN:OD1	2.35	0.58
1:E:484:ASP:OD2	2:F:92:ARG:NH2	2.36	0.58
1:C:131:LYS:NZ	1:C:135:GLU:OE1	2.34	0.58
1:C:378:GLU:OE1	1:C:390:GLN:NE2	2.37	0.57
1:E:204:LYS:O	1:E:206:GLU:HB3	2.05	0.57
1:A:222:ARG:NH2	1:A:253:GLU:OE2	2.38	0.57
1:A:504:ASN:HD22	1:A:538:LEU:HD21	1.70	0.56
1:G:423:ILE:HG22	1:G:427:LYS:HB2	1.87	0.56
2:H:126:ASN:ND2	2:H:126:ASN:O	2.39	0.56
1:C:449:GLN:OE1	2:D:56:ALA:N	2.38	0.56
1:G:393:ARG:NH2	1:G:397:ASN:OD1	2.38	0.56
1:G:201:LYS:NZ	1:G:207:GLN:OE1	2.39	0.56
1:A:131:LYS:HG3	1:A:156:ILE:HG21	1.88	0.56
2:D:31:ALA:HA	5:D:301:GNP:H5'2	1.88	0.55
1:C:155:LYS:NZ	1:C:217:ASP:OD2	2.28	0.55
1:E:51:LEU:HB2	1:E:95:ILE:HG21	1.88	0.55
1:G:116:ASP:O	1:G:120:ASN:ND2	2.40	0.55
1:A:106:ASN:ND2	1:A:111:PHE:O	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:67:ASP:OD1	2:B:67:ASP:N	2.39	0.54
1:E:209:GLU:OE2	1:E:258:GLN:NE2	2.39	0.54
2:H:23:LYS:HB3	2:H:94:ALA:HA	1.90	0.54
2:F:102:ASP:OD2	2:F:104:THR:OG1	2.23	0.54
1:A:280:ASN:OD1	1:A:281:ALA:N	2.41	0.54
2:D:42:VAL:HG22	2:D:61:GLN:HB2	1.90	0.53
1:C:457:GLN:HG3	2:D:58:PHE:HE1	1.74	0.53
1:G:500:ILE:HG22	1:G:538:LEU:HD23	1.89	0.53
1:E:357:SER:O	4:E:602:GOL:O1	2.25	0.53
1:G:434:ASP:OD1	1:G:437:SER:N	2.40	0.53
1:C:423:ILE:N	1:C:424:GLY:HA2	2.24	0.53
1:E:18:SER:HB2	1:E:428:LEU:HD23	1.90	0.53
1:G:98:LEU:HD11	1:G:103:LEU:HD11	1.90	0.53
1:A:190:ASP:O	1:A:194:ASN:ND2	2.42	0.52
1:G:357:SER:OG	1:G:512:GLU:OE2	2.25	0.52
1:A:238:VAL:HG21	1:A:264:VAL:HB	1.91	0.52
2:H:26:LEU:O	2:H:77:THR:OG1	2.24	0.52
1:C:421:LEU:O	1:C:502:GLN:NE2	2.34	0.52
1:A:478:GLU:HG3	1:A:492:LYS:HE3	1.92	0.52
1:C:461:GLU:OE2	2:D:71:LYS:NZ	2.31	0.52
2:D:129:ILE:HB	2:D:158:LEU:HD22	1.91	0.52
1:E:103:LEU:HD22	1:E:121:ILE:HG13	1.92	0.52
1:E:343:VAL:HG23	1:E:344:GLU:HG3	1.92	0.52
1:E:426:ASP:N	1:E:426:ASP:OD2	2.43	0.52
1:G:18:SER:HB2	1:G:428:LEU:HD23	1.92	0.52
1:C:215:LEU:HB3	1:C:253:GLU:HA	1.92	0.52
2:B:142:ARG:NH2	2:B:162:GLU:OE2	2.41	0.52
1:G:545:VAL:HG23	1:G:546:VAL:HG13	1.92	0.52
1:G:484:ASP:OD2	2:H:92:ARG:NH2	2.43	0.52
1:C:457:GLN:HG3	2:D:58:PHE:CE1	2.45	0.52
1:G:309:VAL:HG22	1:G:372:ILE:HB	1.91	0.52
1:A:387:THR:HG23	1:A:390:GLN:H	1.74	0.51
1:G:250:ARG:HD2	3:G:601:EDO:O2	2.10	0.51
1:E:457:GLN:HG3	2:F:58:PHE:CE1	2.45	0.51
1:C:373:TYR:O	1:C:401:GLN:HG2	2.10	0.51
1:G:390:GLN:HA	1:G:393:ARG:HB2	1.91	0.51
1:A:116:ASP:OD2	1:A:119:ARG:NH2	2.44	0.51
1:G:51:LEU:HB2	1:G:95:ILE:HG21	1.93	0.51
1:G:382:THR:OG1	1:G:383:ASN:N	2.43	0.51
1:G:129:GLN:O	1:G:133:HIS:ND1	2.40	0.51
1:C:556:PHE:HD1	1:C:556:PHE:H	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:330:GLU:HA	1:G:333:SER:HB3	1.93	0.51
1:A:373:TYR:O	1:A:401:GLN:HG2	2.11	0.51
2:B:37:LEU:HD23	2:B:165:ALA:HB2	1.92	0.51
1:E:364:VAL:HG13	1:E:502:GLN:HG2	1.91	0.51
2:F:80:LEU:HD12	2:F:83:TYR:HE2	1.76	0.51
2:D:170:ASN:HA	2:D:173:GLU:HB2	1.91	0.51
1:E:482:THR:HG23	1:E:483:VAL:HG23	1.93	0.51
1:G:166:ALA:HB1	1:G:188:LYS:HB3	1.93	0.50
1:A:271:HIS:ND1	1:A:272:PRO:HD2	2.26	0.50
2:D:34:LYS:NZ	5:D:301:GNP:O1B	2.37	0.50
1:A:412:THR:O	1:A:548:LEU:HD11	2.12	0.50
1:C:18:SER:HB2	1:C:428:LEU:HD23	1.92	0.50
1:E:372:ILE:HG12	1:E:405:LEU:HD22	1.93	0.50
1:G:387:THR:O	1:G:390:GLN:HG2	2.11	0.50
2:H:38:VAL:HG11	2:H:59:LEU:HD13	1.92	0.50
1:A:362:GLU:OE2	1:A:501:LYS:NZ	2.40	0.50
1:E:94:LEU:HD11	1:E:125:ILE:HD13	1.94	0.50
1:G:368:ILE:H	1:G:368:ILE:HD12	1.77	0.50
2:B:164:SER:HB3	2:B:169:MET:HB3	1.94	0.50
2:D:23:LYS:HB3	2:D:94:ALA:HA	1.94	0.50
1:C:278:GLY:O	1:C:286:ILE:N	2.44	0.49
2:B:40:ARG:HG2	2:B:171:VAL:HG21	1.94	0.49
1:G:120:ASN:HB3	1:G:193:LEU:HD12	1.94	0.49
1:E:372:ILE:HD13	1:E:402:THR:HG23	1.94	0.49
2:H:34:LYS:NZ	5:H:301:GNP:O3G	2.40	0.49
1:A:215:LEU:HD13	1:A:261:ILE:HG12	1.95	0.49
1:E:401:GLN:NE2	1:E:404:GLN:OE1	2.46	0.49
2:H:57:ALA:HB3	2:H:76:ASP:HB3	1.94	0.49
1:C:184:LYS:H	1:C:184:LYS:HD2	1.78	0.48
1:A:28:TYR:CE1	1:A:416:PRO:HD3	2.48	0.48
1:C:368:ILE:H	1:C:368:ILE:HD12	1.76	0.48
1:E:383:ASN:OD1	1:E:384:THR:N	2.46	0.48
1:G:372:ILE:HD13	1:G:402:THR:HG23	1.95	0.48
1:A:30:VAL:HG22	1:A:411:GLN:HB2	1.95	0.48
1:C:366:TYR:HB2	1:C:422:TYR:CE2	2.49	0.48
1:E:437:SER:HB2	1:E:438:GLU:HB2	1.96	0.48
1:G:33:PRO:HG3	1:G:409:HIS:HB3	1.96	0.47
1:A:177:ILE:HG22	1:A:181:LYS:HE2	1.95	0.47
1:G:332:ILE:O	1:G:336:LYS:N	2.44	0.47
1:C:378:GLU:HG3	1:C:378:GLU:H	1.48	0.47
1:G:271:HIS:ND1	1:G:272:PRO:HD2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:205:GLY:N	1:G:206:GLU:OE1	2.42	0.47
1:E:368:ILE:HD12	1:E:368:ILE:H	1.80	0.47
2:H:27:LEU:HD12	2:H:119:LEU:HD11	1.96	0.47
1:C:461:GLU:OE1	1:C:469:SER:OG	2.33	0.47
2:H:42:VAL:HG12	2:H:43:LYS:HG3	1.96	0.47
1:C:120:ASN:HB3	1:C:193:LEU:HD12	1.96	0.47
1:C:100:ILE:HD12	1:C:100:ILE:H	1.80	0.46
1:E:338:ARG:NH1	1:E:519:GLU:OE2	2.49	0.46
2:D:113:LYS:HG2	2:D:152:TYR:CZ	2.50	0.46
1:C:59:GLU:OE2	1:C:399:TYR:OH	2.27	0.46
2:B:23:LYS:HA	2:B:73:GLU:HB2	1.97	0.46
1:A:202:GLY:O	1:A:205:GLY:N	2.45	0.46
1:C:387:THR:O	1:C:390:GLN:HG2	2.16	0.46
1:G:457:GLN:HG3	2:H:58:PHE:CE1	2.45	0.46
1:G:312:GLU:O	1:G:376:THR:OG1	2.33	0.46
1:A:214:THR:HA	1:A:260:SER:HA	1.97	0.46
2:D:33:GLY:HA3	2:D:134:ASN:ND2	2.31	0.46
1:A:312:GLU:OE2	1:A:320:ARG:NH1	2.49	0.46
1:G:343:VAL:HA	1:G:344:GLU:HA	1.55	0.46
2:F:46:PHE:O	2:F:47:HIS:ND1	2.49	0.46
1:C:469:SER:HB3	2:D:21:GLN:HE22	1.81	0.45
1:A:417:LEU:HD12	1:A:485:ALA:HB2	1.97	0.45
1:C:311:ALA:HB1	1:C:376:THR:HG23	1.97	0.45
1:E:271:HIS:ND1	1:E:272:PRO:HD2	2.31	0.45
1:E:28:TYR:CE1	1:E:416:PRO:HD3	2.52	0.45
1:G:222:ARG:NH2	1:G:253:GLU:OE2	2.48	0.45
1:A:457:GLN:HG3	2:B:58:PHE:CE1	2.48	0.45
1:C:310:LYS:HD3	1:C:373:TYR:HE1	1.82	0.45
1:G:196:ILE:O	1:G:212:ARG:NH1	2.42	0.45
1:G:172:ASN:OD1	1:G:173:VAL:N	2.50	0.45
1:E:449:GLN:OE1	2:F:56:ALA:N	2.50	0.45
1:G:437:SER:HA	1:G:438:GLU:HA	1.84	0.45
2:D:21:GLN:HG2	2:D:71:LYS:HB3	1.98	0.45
1:C:304:GLU:HB3	1:C:368:ILE:HD13	2.00	0.45
1:C:238:VAL:HG23	1:C:251:TYR:HB2	1.99	0.45
1:A:482:THR:HG23	1:A:483:VAL:HG23	1.98	0.45
1:C:270:ALA:O	1:C:288:ASP:N	2.50	0.45
1:A:127:MET:O	1:A:131:LYS:HB2	2.17	0.44
1:G:541:PRO:O	1:G:544:TRP:HD1	2.00	0.44
1:G:58:GLN:HG2	1:G:88:ILE:HD12	2.00	0.44
1:G:373:TYR:O	1:G:401:GLN:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:359:LEU:HD22	1:G:359:LEU:HA	1.80	0.44
1:A:254:ASP:OD1	1:A:254:ASP:N	2.51	0.44
2:B:127:ILE:HG23	2:B:129:ILE:HG13	1.99	0.44
1:G:206:GLU:N	1:G:206:GLU:OE1	2.48	0.44
1:G:490:ILE:HD12	1:G:550:LYS:HA	2.00	0.44
1:E:343:VAL:HA	1:E:344:GLU:HA	1.51	0.44
1:C:376:THR:HB	1:C:380:THR:OG1	2.17	0.44
1:G:109:VAL:HA	1:G:110:GLY:HA3	1.47	0.44
1:A:552:PRO:O	1:A:554:GLN:N	2.44	0.44
1:A:309:VAL:HG22	1:A:372:ILE:HB	2.00	0.44
1:E:151:ILE:O	1:E:155:LYS:HG3	2.18	0.44
2:B:152:TYR:O	2:B:156:ASN:ND2	2.33	0.44
1:C:123:ASP:HB3	1:C:159:TYR:HE2	1.83	0.43
1:E:139:GLN:HG2	1:E:141:ILE:HG13	2.00	0.43
2:B:66:ASP:OD1	2:B:67:ASP:N	2.51	0.43
1:C:192:ALA:O	1:C:195:SER:OG	2.30	0.43
1:E:84:VAL:HG13	1:E:129:GLN:HG2	1.99	0.43
2:B:42:VAL:HA	2:B:61:GLN:HE21	1.83	0.43
1:G:141:ILE:HA	1:G:142:PRO:HD2	1.87	0.43
1:A:332:ILE:HD13	1:A:556:PHE:HA	1.99	0.43
1:A:372:ILE:HD13	1:A:402:THR:HG23	1.99	0.43
1:E:107:SER:HA	1:E:108:GLY:HA2	1.71	0.43
2:F:47:HIS:HB2	2:F:50:GLN:HG3	1.99	0.43
1:G:491:GLN:HA	1:G:494:LYS:HD3	2.00	0.43
1:G:366:TYR:HB2	1:G:422:TYR:CE2	2.53	0.43
1:A:214:THR:OG1	1:A:217:ASP:OD1	2.30	0.43
1:A:378:GLU:O	1:A:383:ASN:ND2	2.50	0.43
1:C:488:ASP:OD1	1:C:489:ASP:N	2.51	0.43
2:F:64:CYS:SG	2:H:69:THR:OG1	2.75	0.43
1:E:166:ALA:HB1	1:E:188:LYS:HB3	2.01	0.43
1:C:486:LYS:HD2	1:C:486:LYS:H	1.83	0.43
1:C:416:PRO:O	1:C:420:ILE:HG12	2.18	0.43
1:C:134:LEU:HA	1:C:134:LEU:HD23	1.82	0.43
1:E:123:ASP:HB3	1:E:159:TYR:HE2	1.83	0.43
2:B:35:SER:OG	2:B:76:ASP:OD2	2.36	0.43
2:D:147:GLN:HA	2:D:150:GLN:HB3	2.00	0.43
1:E:30:VAL:HG22	1:E:411:GLN:HB2	2.01	0.42
1:G:295:MET:SD	1:G:308:CYS:HB3	2.59	0.42
1:E:437:SER:HA	1:E:438:GLU:HA	1.78	0.42
1:A:547:SER:OG	1:A:548:LEU:N	2.53	0.42
1:E:134:LEU:HA	1:E:134:LEU:HD23	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:GLN:HE21	2:B:50:GLN:HB3	1.69	0.42
1:G:134:LEU:HD12	1:G:156:ILE:HD12	2.02	0.42
1:C:93:LYS:NZ	1:C:174:ASP:OD2	2.43	0.42
1:E:94:LEU:HD23	1:E:173:VAL:HG13	2.02	0.42
1:C:125:ILE:HG12	1:C:176:ILE:HD13	2.01	0.42
1:A:415:HIS:CG	1:A:416:PRO:HD2	2.54	0.42
1:G:489:ASP:HA	1:G:492:LYS:NZ	2.34	0.42
2:F:165:ALA:N	5:F:301:GNP:O6	2.50	0.42
1:E:545:VAL:HG23	1:E:546:VAL:HG13	2.02	0.42
1:C:222:ARG:O	1:C:230:LYS:NZ	2.49	0.42
1:E:396:LYS:HE2	1:E:396:LYS:HB3	1.84	0.42
1:C:22:LYS:HG2	1:C:28:TYR:CE2	2.55	0.42
2:B:176:MET:O	2:B:180:LYS:HG2	2.20	0.42
1:G:117:ARG:O	1:G:121:ILE:HG12	2.20	0.41
2:F:26:LEU:O	2:F:77:THR:OG1	2.27	0.41
1:C:210:ASN:HA	1:C:211:PRO:HD2	1.87	0.41
2:D:142:ARG:HH22	2:D:162:GLU:CD	2.24	0.41
1:A:245:LYS:NZ	3:A:602:EDO:H22	2.35	0.41
1:E:476:GLN:O	1:E:480:ILE:HG13	2.21	0.41
1:C:51:LEU:HD21	1:C:92:LYS:HA	2.01	0.41
1:E:364:VAL:HG12	1:E:365:TYR:CD2	2.55	0.41
2:F:69:THR:OG1	2:H:64:CYS:SG	2.71	0.41
1:A:385:SER:HA	1:A:386:PRO:HD3	1.84	0.41
1:A:123:ASP:HB3	1:A:159:TYR:HE2	1.84	0.41
1:C:449:GLN:HE21	1:C:449:GLN:HB2	1.64	0.41
1:G:522:ALA:HB2	1:G:529:SER:HB2	2.02	0.41
2:D:135:LYS:HG2	5:D:301:GNP:C5	2.50	0.41
1:A:480:ILE:HD11	3:B:303:EDO:H11	2.03	0.41
1:C:415:HIS:HB2	1:C:491:GLN:NE2	2.35	0.41
1:G:434:ASP:O	2:H:82:ARG:NH2	2.54	0.41
1:G:184:LYS:HD2	1:G:184:LYS:H	1.85	0.41
1:G:319:ASP:OD1	1:G:323:LYS:NZ	2.53	0.41
1:A:141:ILE:HA	1:A:142:PRO:HD2	1.68	0.41
1:C:415:HIS:CG	1:C:416:PRO:HD2	2.56	0.41
1:C:447:HIS:ND1	1:C:485:ALA:HB2	2.35	0.41
1:E:500:ILE:HD13	1:E:534:ILE:HG23	2.02	0.41
1:E:142:PRO:HA	1:E:143:PRO:HD3	1.83	0.41
1:C:271:HIS:CG	1:C:272:PRO:HD2	2.56	0.41
1:E:182:SER:OG	1:E:184:LYS:HD2	2.21	0.41
2:D:34:LYS:NZ	5:D:301:GNP:O3G	2.40	0.41
1:E:498:LEU:O	1:E:502:GLN:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:80:LEU:HB2	2:F:83:TYR:CD2	2.56	0.41
2:D:142:ARG:NH1	2:D:144:VAL:O	2.52	0.41
1:C:454:LEU:O	1:C:458:ILE:HG13	2.21	0.41
1:E:48:ILE:HG12	1:E:48:ILE:H	1.61	0.41
2:D:92:ARG:NH1	2:D:92:ARG:HB3	2.36	0.41
1:C:548:LEU:HD12	1:C:548:LEU:HA	1.79	0.41
1:C:48:ILE:H	1:C:48:ILE:HG12	1.70	0.41
2:D:174:ILE:O	2:D:178:ILE:HG13	2.20	0.41
1:C:313:ALA:O	1:C:317:PHE:N	2.50	0.41
1:E:393:ARG:HG2	1:E:396:LYS:HE2	2.02	0.40
1:C:204:LYS:HA	1:C:204:LYS:HD2	1.88	0.40
1:G:60:ARG:HD2	1:G:406:LEU:HD23	2.03	0.40
1:C:90:ASP:HB3	1:C:173:VAL:HG21	2.03	0.40
1:E:271:HIS:CD2	1:E:273:VAL:HB	2.57	0.40
1:C:166:ALA:HB1	1:C:188:LYS:HB3	2.04	0.40
1:C:552:PRO:O	1:C:554:GLN:N	2.53	0.40
2:F:42:VAL:HA	2:F:61:GLN:HE21	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	526/551 (96%)	508 (97%)	16 (3%)	2 (0%)	39	75
1	C	523/551 (95%)	505 (97%)	17 (3%)	1 (0%)	52	84
1	E	525/551 (95%)	503 (96%)	20 (4%)	2 (0%)	39	75
1	G	522/551 (95%)	499 (96%)	22 (4%)	1 (0%)	52	84
2	B	162/170 (95%)	152 (94%)	10 (6%)	0	100	100
2	D	162/170 (95%)	152 (94%)	8 (5%)	2 (1%)	16	53
2	F	162/170 (95%)	151 (93%)	11 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	162/170 (95%)	149 (92%)	13 (8%)	0	100	100
All	All	2744/2884 (95%)	2619 (95%)	117 (4%)	8 (0%)	46	80

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	382	THR
1	G	106	ASN
1	A	553	ALA
2	D	92	ARG
1	E	552	PRO
2	D	55	GLY
1	E	205	GLY
1	A	379	VAL

5.3.2 Protein sidechains ⓘ

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	451/466 (97%)	425 (94%)	26 (6%)	25	61
1	C	448/466 (96%)	413 (92%)	35 (8%)	16	50
1	E	452/466 (97%)	417 (92%)	35 (8%)	16	50
1	G	449/466 (96%)	422 (94%)	27 (6%)	24	60
2	B	134/137 (98%)	132 (98%)	2 (2%)	72	90
2	D	134/137 (98%)	132 (98%)	2 (2%)	72	90
2	F	134/137 (98%)	132 (98%)	2 (2%)	72	90
2	H	134/137 (98%)	130 (97%)	4 (3%)	48	81
All	All	2336/2412 (97%)	2203 (94%)	133 (6%)	25	62

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	VAL
1	A	39	VAL
1	A	48	ILE
1	A	51	LEU
1	A	55	GLN
1	A	88	ILE
1	A	158	LEU
1	A	171	ASN
1	A	184	LYS
1	A	204	LYS
1	A	209	GLU
1	A	215	LEU
1	A	221	LEU
1	A	254	ASP
1	A	295	MET
1	A	342	LEU
1	A	343	VAL
1	A	381	THR
1	A	393	ARG
1	A	403	MET
1	A	406	LEU
1	A	417	LEU
1	A	426	ASP
1	A	449	GLN
1	A	490	ILE
1	A	492	LYS
2	B	137	ASP
2	B	159	LEU
1	C	48	ILE
1	C	62	LYS
1	C	94	LEU
1	C	127	MET
1	C	134	LEU
1	C	158	LEU
1	C	165	ARG
1	C	171	ASN
1	C	179	LEU
1	C	218	LEU
1	C	238	VAL
1	C	248	LEU
1	C	254	ASP
1	C	304	GLU
1	C	338	ARG

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Mol	Chain	Res	Type
1	C	358	VAL
1	C	378	GLU
1	C	380	THR
1	C	387	THR
1	C	393	ARG
1	C	403	MET
1	C	406	LEU
1	C	417	LEU
1	C	430	ASP
1	C	435	GLU
1	C	439	LYS
1	C	449	GLN
1	C	464	ASP
1	C	479	ASP
1	C	486	LYS
1	C	490	ILE
1	C	496	PHE
1	C	538	LEU
1	C	550	LYS
1	C	556	PHE
2	D	92	ARG
2	D	159	LEU
1	E	39	VAL
1	E	48	ILE
1	E	62	LYS
1	E	77	MET
1	E	94	LEU
1	E	100	ILE
1	E	112	ARG
1	E	158	LEU
1	E	184	LYS
1	E	186	LEU
1	E	204	LYS
1	E	206	GLU
1	E	207	GLN
1	E	215	LEU
1	E	218	LEU
1	E	221	LEU
1	E	250	ARG
1	E	254	ASP
1	E	266	GLN
1	E	295	MET

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Mol	Chain	Res	Type
1	E	304	GLU
1	E	357	SER
1	E	363	LYS
1	E	364	VAL
1	E	380	THR
1	E	381	THR
1	E	382	THR
1	E	389	GLU
1	E	401	GLN
1	E	403	MET
1	E	417	LEU
1	E	426	ASP
1	E	439	LYS
1	E	449	GLN
1	E	557	LYS
2	F	59	LEU
2	F	141	LYS
1	G	41	SER
1	G	94	LEU
1	G	127	MET
1	G	141	ILE
1	G	179	LEU
1	G	209	GLU
1	G	221	LEU
1	G	248	LEU
1	G	294	ASN
1	G	295	MET
1	G	336	LYS
1	G	359	LEU
1	G	364	VAL
1	G	376	THR
1	G	384	THR
1	G	393	ARG
1	G	403	MET
1	G	405	LEU
1	G	417	LEU
1	G	425	HIS
1	G	426	ASP
1	G	429	LYS
1	G	479	ASP
1	G	490	ILE
1	G	496	PHE

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Mol	Chain	Res	Type
1	G	544	TRP
1	G	556	PHE
2	H	19	ILE
2	H	54	ILE
2	H	82	ARG
2	H	126	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	390	GLN
1	C	172	ASN
1	C	271	HIS
2	D	95	GLN
1	E	401	GLN
1	E	411	GLN
2	F	61	GLN
1	G	139	GLN
1	G	411	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 4 are monoatomic - leaving 13 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	A	601	-	3,3,3	0.47	0	2,2,2	0.45	0
3	EDO	A	602	-	3,3,3	0.47	0	2,2,2	0.41	0
4	GOL	A	603	-	5,5,5	0.33	0	5,5,5	0.23	0
4	GOL	A	604	-	5,5,5	0.35	0	5,5,5	0.26	0
5	GNP	B	301	6	28,34,34	1.89	4 (14%)	33,54,54	2.37	7 (21%)
3	EDO	B	302	-	3,3,3	0.45	0	2,2,2	0.42	0
3	EDO	B	303	-	3,3,3	0.46	0	2,2,2	0.48	0
5	GNP	D	301	6	28,34,34	1.89	5 (17%)	33,54,54	2.36	7 (21%)
3	EDO	E	601	-	3,3,3	0.47	0	2,2,2	0.42	0
4	GOL	E	602	-	5,5,5	0.35	0	5,5,5	0.26	0
5	GNP	F	301	6	28,34,34	1.89	4 (14%)	33,54,54	2.34	7 (21%)
3	EDO	G	601	-	3,3,3	0.46	0	2,2,2	0.44	0
5	GNP	H	301	6	28,34,34	1.90	6 (21%)	33,54,54	2.38	7 (21%)

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
3	EDO	A	601	-	-	0/1/1/1	0/0/0/0
3	EDO	A	602	-	-	0/1/1/1	0/0/0/0
4	GOL	A	603	-	-	0/4/4/4	0/0/0/0
4	GOL	A	604	-	-	0/4/4/4	0/0/0/0
5	GNP	B	301	6	-	1/12/38/38	0/3/3/3
3	EDO	B	302	-	-	0/1/1/1	0/0/0/0
3	EDO	B	303	-	-	0/1/1/1	0/0/0/0
5	GNP	D	301	6	-	0/12/38/38	0/3/3/3
3	EDO	E	601	-	-	0/1/1/1	0/0/0/0
4	GOL	E	602	-	-	0/4/4/4	0/0/0/0
5	GNP	F	301	6	-	0/12/38/38	0/3/3/3
3	EDO	G	601	-	-	0/1/1/1	0/0/0/0
5	GNP	H	301	6	-	0/12/38/38	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	301	GNP	PB-O3A	-5.46	1.52	1.59
5	F	301	GNP	PB-O3A	-5.37	1.52	1.59
5	D	301	GNP	PB-O3A	-5.32	1.52	1.59
5	B	301	GNP	PB-O3A	-5.31	1.52	1.59
5	B	301	GNP	PB-O2B	-3.10	1.48	1.56
5	H	301	GNP	PB-O2B	-3.08	1.48	1.56
5	D	301	GNP	PB-O2B	-3.08	1.48	1.56
5	F	301	GNP	PB-O2B	-3.00	1.48	1.56
5	D	301	GNP	C8-N7	-2.03	1.30	1.34
5	H	301	GNP	C8-N7	-2.03	1.30	1.34
5	H	301	GNP	PG-O3G	-2.00	1.51	1.56
5	F	301	GNP	C6-N1	3.45	1.39	1.33
5	B	301	GNP	C6-N1	3.45	1.39	1.33
5	H	301	GNP	C6-N1	3.52	1.39	1.33
5	D	301	GNP	C6-N1	3.57	1.39	1.33
5	H	301	GNP	PG-O1G	4.49	1.51	1.46
5	D	301	GNP	PG-O1G	4.52	1.51	1.46
5	F	301	GNP	PG-O1G	4.54	1.51	1.46
5	B	301	GNP	PG-O1G	4.60	1.51	1.46

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	301	GNP	C5-C6-N1	-8.72	111.67	123.59
5	D	301	GNP	C5-C6-N1	-8.69	111.71	123.59
5	B	301	GNP	C5-C6-N1	-8.65	111.76	123.59
5	F	301	GNP	C5-C6-N1	-8.54	111.91	123.59
5	D	301	GNP	PA-O3A-PB	-3.61	120.58	132.67
5	H	301	GNP	PA-O3A-PB	-3.55	120.78	132.67
5	B	301	GNP	PA-O3A-PB	-3.50	120.93	132.67
5	F	301	GNP	PA-O3A-PB	-3.45	121.09	132.67
5	H	301	GNP	O3G-PG-O1G	-3.26	104.83	113.49
5	B	301	GNP	O3G-PG-O1G	-3.26	104.83	113.49
5	D	301	GNP	O3G-PG-O1G	-3.18	105.03	113.49
5	F	301	GNP	O3G-PG-O1G	-3.14	105.14	113.49
5	H	301	GNP	N3-C2-N1	-2.18	124.12	127.44
5	B	301	GNP	N3-C2-N1	-2.17	124.14	127.44
5	F	301	GNP	N3-C2-N1	-2.16	124.16	127.44
5	D	301	GNP	N3-C2-N1	-2.12	124.22	127.44
5	B	301	GNP	O3G-PG-O2G	2.78	115.83	107.58
5	D	301	GNP	O3G-PG-O2G	2.81	115.92	107.58
5	F	301	GNP	O3G-PG-O2G	2.84	116.00	107.58
5	H	301	GNP	O3G-PG-O2G	2.91	116.21	107.58

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
5	D	301	GNP	O2B-PB-O1B	3.80	117.93	110.00
5	F	301	GNP	O2B-PB-O1B	3.83	118.00	110.00
5	B	301	GNP	O2B-PB-O1B	3.89	118.11	110.00
5	H	301	GNP	O2B-PB-O1B	3.95	118.24	110.00
5	F	301	GNP	C6-N1-C2	6.30	124.68	115.94
5	D	301	GNP	C6-N1-C2	6.30	124.69	115.94
5	B	301	GNP	C6-N1-C2	6.32	124.71	115.94
5	H	301	GNP	C6-N1-C2	6.38	124.79	115.94

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	301	GNP	O1B-PB-N3B-PG

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	EDO	1	0
3	B	303	EDO	1	0
5	D	301	GNP	4	0
4	E	602	GOL	1	0
5	F	301	GNP	1	0
3	G	601	EDO	2	0
5	H	301	GNP	1	0

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	530/551 (96%)	-0.40	1 (0%) 95 90	1, 36, 77, 137	0
1	C	527/551 (95%)	-0.20	16 (3%) 54 28	5, 57, 109, 169	0
1	E	531/551 (96%)	-0.38	2 (0%) 93 84	0, 32, 79, 118	0
1	G	528/551 (95%)	-0.09	24 (4%) 37 17	14, 59, 112, 142	0
2	B	164/170 (96%)	-0.32	0 100 100	16, 58, 89, 151	0
2	D	164/170 (96%)	-0.31	1 (0%) 90 79	25, 73, 108, 133	0
2	F	164/170 (96%)	-0.14	2 (1%) 81 63	22, 72, 108, 149	0
2	H	164/170 (96%)	-0.33	0 100 100	26, 60, 99, 130	0
All	All	2772/2884 (96%)	-0.27	46 (1%) 73 51	0, 52, 102, 169	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	344	GLU	4.8
1	C	26	GLY	4.2
1	G	78	THR	4.2
1	G	77	MET	3.9
1	G	80	SER	3.8
1	G	361	ARG	3.7
1	G	204	LYS	3.5
1	G	203	ALA	3.5
1	G	107	SER	3.4
1	C	47	GLY	3.4
2	F	162	GLU	3.3
1	G	333	SER	3.3
1	G	356	SER	3.3
1	G	74	ALA	3.2
1	C	77	MET	3.2
1	G	75	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	G	108	GLY	3.2
1	G	528	PRO	3.1
1	C	384	THR	3.1
2	F	147	GLN	3.0
1	G	340	ASP	3.0
1	G	536	ASN	3.0
1	G	109	VAL	2.9
1	C	380	THR	2.8
1	G	339	MET	2.8
2	D	22	PHE	2.7
1	G	344	GLU	2.7
1	C	429	LYS	2.6
1	C	203	ALA	2.6
1	G	76	ALA	2.6
1	C	528	PRO	2.4
1	C	556	PHE	2.4
1	C	555	ASP	2.4
1	C	78	THR	2.4
1	C	109	VAL	2.4
1	C	75	GLY	2.3
1	G	360	ASN	2.3
1	E	107	SER	2.3
1	A	144	GLU	2.3
1	G	110	GLY	2.2
1	G	525	ALA	2.2
1	C	439	LYS	2.1
1	G	202	GLY	2.1
1	C	204	LYS	2.1
1	C	76	ALA	2.0
1	G	262	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	EDO	B	303	4/4	0.87	0.32	4.12	41,41,41,41	0
3	EDO	B	302	4/4	0.76	0.42	3.04	45,45,45,45	0
4	GOL	A	604	6/6	0.50	0.42	2.90	78,78,78,78	0
3	EDO	A	602	4/4	0.57	0.31	1.97	55,55,55,55	0
4	GOL	E	602	6/6	0.74	0.27	1.67	66,66,66,66	0
3	EDO	G	601	4/4	0.67	0.35	1.48	84,84,84,84	0
4	GOL	A	603	6/6	0.84	0.25	0.45	59,59,59,59	0
3	EDO	A	601	4/4	0.87	0.21	0.31	58,58,58,58	0
6	MG	F	302	1/1	0.96	0.26	0.17	54,54,54,54	0
6	MG	D	302	1/1	0.99	0.18	0.08	36,36,36,36	0
6	MG	B	304	1/1	0.94	0.20	0.01	36,36,36,36	0
5	GNP	H	301	32/32	0.94	0.16	-0.25	63,63,63,63	0
5	GNP	B	301	32/32	0.89	0.18	-0.51	72,72,72,72	0
5	GNP	F	301	32/32	0.86	0.17	-0.65	81,81,81,81	0
5	GNP	D	301	32/32	0.94	0.15	-0.75	80,80,80,80	0
3	EDO	E	601	4/4	0.87	0.29	-	56,56,56,56	0
6	MG	H	302	1/1	0.98	0.22	-	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.