

Full wwPDB X-ray Structure Validation Report (i)

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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
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 2.55 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	$\begin{array}{c} {\rm Whole \ archive} \\ (\#{\rm Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	$1284 \ (2.56-2.52)$
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	$1315 \ (2.56-2.52)$
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272(2.56-2.52)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain		
1	А	217	80%	15%	5%
1	В	217	% 7 5%	20%	5%
1	С	217	79%	15%	6%
1	D	217	80%	13%	7%
1	Е	217	% • 79%	16%	5%



Mol	Chain	Length	Quality of chain		
1	F	217	8%	16%	7%
1	G	217	80%	14%	6%
1	Н	217	6% 78%	15%	6%



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2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 13204 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	206	Total	С	Ν	0	S	0	0	0
	A	200	1629	1040	280	299	10	0	0	0
1	р	207	Total	С	Ν	0	S	0	0	0
	D	207	1619	1034	283	292	10	0	0	0
1	С	205	Total	С	Ν	0	S	0	0	0
1		200	1633	1042	282	299	10	0	0	0
1	Л	202	Total	С	Ν	0	S	0	0	0
1	D	202	1607	1028	276	293	10		0	0
1	F	207	Total	С	Ν	0	S	0	0	0
L	Ľ	201	1658	1058	288	302	10	0	0	0
1	F	202	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
1	I.	202	1584	1011	273	290	10	0	0	0
1	C	203	Total	С	Ν	0	\mathbf{S}	0	0	0
1	G	203	1620	1035	280	296	9	0	0	0
1	Ц	203	Total	С	Ν	0	S	0	0	0
	11	203	1560	997	268	285	10	U	0	

• Molecule 1 is a protein called Glycolipid transfer protein domain-containing protein 1.

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	0	SER	-	expression tag	UNP Q8BS40
А	77	THR	ALA	conflict	UNP Q8BS40
В	0	SER	-	expression tag	UNP Q8BS40
В	77	THR	ALA	conflict	UNP Q8BS40
С	0	SER	-	expression tag	UNP Q8BS40
С	77	THR	ALA	conflict	UNP Q8BS40
D	0	SER	-	expression tag	UNP Q8BS40
D	77	THR	ALA	conflict	UNP Q8BS40
Е	0	SER	-	expression tag	UNP Q8BS40
Е	77	THR	ALA	conflict	UNP Q8BS40
F	0	SER	-	expression tag	UNP Q8BS40
F	77	THR	ALA	conflict	UNP Q8BS40
G	0	SER	-	expression tag	UNP Q8BS40



Continuea from previous page								
Chain	Residue	Modelled	Actual	Comment	Reference			
G	77	THR	ALA	conflict	UNP Q8BS40			
Н	0	SER	-	expression tag	UNP Q8BS40			
Н	77	THR	ALA	conflict	UNP Q8BS40			

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• Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
2	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
2	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
2	Е	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
2	F	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
2	G	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
2	Н	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 3 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	54	$\begin{array}{cc} \text{Total} & \text{O} \\ 54 & 54 \end{array}$	0	0
3	В	38	Total O 38 38	0	0
3	С	46	Total O 46 46	0	0
3	D	15	Total O 15 15	0	0
3	Ε	35	$\begin{array}{cc} \text{Total} & \text{O} \\ 35 & 35 \end{array}$	0	0
3	F	15	Total O 15 15	0	0
3	G	29	TotalO2929	0	0
3	Н	22	TotalO2222	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Glycolipid transfer protein domain-containing protein 1



8169 F173 M179 M179 G183 G184 G184 G184 A185 F195 L206 L206 L212 L215 L215

• Molecule 1: Glycolipid transfer protein domain-containing protein 1





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	82.00Å 83.88Å 268.72Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	39.51 - 2.55	Depositor
Resolution (A)	49.06 - 2.55	EDS
% Data completeness	93.3 (39.51-2.55)	Depositor
(in resolution range)	93.4(49.06-2.55)	EDS
R _{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$3.51 (at 2.54 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
D D.	0.201 , 0.271	Depositor
n, n_{free}	0.201 , 0.271	DCC
R_{free} test set	2915 reflections $(5.06%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	45.8	Xtriage
Anisotropy	0.574	Xtriage
Bulk solvent $k_{sol}(e/A^3)$, $B_{sol}(A^2)$	0.32 , 38.3	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.028 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13204	wwPDB-VP
Average B, all atoms $(Å^2)$	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 15.12% 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: PO4

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

Mal	Chain	Bond	lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.45	0/1665	0.58	0/2256	
1	В	0.45	0/1655	0.60	0/2246	
1	С	0.47	0/1668	0.61	0/2258	
1	D	0.41	0/1642	0.58	0/2223	
1	Е	0.45	0/1695	0.60	0/2294	
1	F	0.38	0/1615	0.54	0/2185	
1	G	0.41	0/1654	0.58	0/2238	
1	Н	0.42	0/1590	0.56	0/2156	
All	All	0.43	0/13184	0.58	0/17856	

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	1629	0	1602	22	0
1	В	1619	0	1592	30	0
1	С	1633	0	1619	21	0
1	D	1607	0	1593	15	0
1	Е	1658	0	1650	28	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1584	0	1573	21	0
1	G	1620	0	1618	17	0
1	Н	1560	0	1526	24	0
2	А	5	0	0	0	0
2	В	5	0	0	0	0
2	С	5	0	0	0	0
2	D	5	0	0	0	0
2	Е	5	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	Н	5	0	0	1	0
3	А	54	0	0	2	0
3	В	38	0	0	0	0
3	С	46	0	0	3	0
3	D	15	0	0	0	0
3	Ε	35	0	0	2	0
3	F	15	0	0	1	0
3	G	29	0	0	0	0
3	Н	22	0	0	1	0
All	All	13204	0	12773	167	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 (167) 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 (Å)	overlap (Å)
1:D:39:LEU:HD13	1:D:120:LEU:HD23	1.66	0.76
1:E:99:HIS:N	3:E:415:HOH:O	2.21	0.74
1:F:14:LEU:HD22	1:F:196:ILE:HD11	1.70	0.73
1:A:14:LEU:HD22	1:A:196:ILE:HD11	1.69	0.73
1:F:51:SER:HA	1:F:54:SER:HB3	1.71	0.73
1:F:39:LEU:HD13	1:F:120:LEU:HD23	1.71	0.70
1:E:37:LYS:NZ	3:E:410:HOH:O	2.24	0.70
1:E:39:LEU:HD13	1:E:120:LEU:HD23	1.74	0.69
1:F:60:LYS:HE2	1:F:112:ARG:HG2	1.76	0.67
1:B:179:MET:HG3	1:B:185:ALA:HA	1.77	0.66
1:D:14:LEU:HD22	1:D:196:ILE:HD11	1.79	0.65
1:D:60:LYS:HE2	1:D:112:ARG:HG2	1.78	0.64
1:E:14:LEU:HD22	1:E:196:ILE:HD11	1.81	0.62
1:C:101:ARG:N	3:C:439:HOH:O	2.32	0.62



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:39:LEU:HD13	1:A:120:LEU:HD23	1.81	0.61	
1:G:14:LEU:HD22	1:G:196:ILE:HD11	1.81	0.61	
1:B:149:ALA:HB1	1:B:157:ARG:HD3	1.82	0.61	
1:E:212:LEU:HD22	1:E:215:LEU:HD11	1.83	0.60	
1:A:163:ALA:HB1	1:C:162:VAL:HG12	1.84	0.59	
1:F:179:MET:HG3	1:F:185:ALA:HA	1.85	0.58	
1:A:12:VAL:O	1:A:15:VAL:HG12	2.03	0.57	
1:B:14:LEU:HD22	1:B:196:ILE:HD11	1.84	0.57	
1:B:162:VAL:HG11	1:E:49:VAL:HA	1.86	0.57	
1:F:60:LYS:HA	1:F:63:ILE:HD12	1.88	0.56	
1:H:14:LEU:HD22	1:H:196:ILE:HD11	1.86	0.56	
1:H:95:ASP:O	1:H:216:PRO:HG3	2.06	0.56	
1:C:36:TRP:HB3	1:C:61:LEU:HD11	1.89	0.55	
1:E:39:LEU:HD22	1:E:120:LEU:HD21	1.88	0.55	
1:B:52:PHE:CE2	1:B:160:VAL:HG22	2.42	0.55	
1:G:9:ASN:HB2	1:G:179:MET:CE	2.37	0.55	
1:G:179:MET:HG3	1:G:185:ALA:HA	1.89	0.55	
1:F:212:LEU:O	1:F:215:LEU:HG	2.06	0.54	
1:H:179:MET:HG3	1:H:185:ALA:HA	1.89	0.54	
1:A:179:MET:HG3	1:A:185:ALA:HA	1.89	0.53	
1:C:179:MET:HG3	1:C:185:ALA:HA	1.90	0.53	
1:E:179:MET:HG3	1:E:185:ALA:HA	1.89	0.53	
1:A:9:ASN:HB2	1:A:179:MET:CE	2.38	0.53	
1:H:39:LEU:HD13	1:H:120:LEU:HD23	1.89	0.53	
1:D:179:MET:HG3	1:D:185:ALA:HA	1.91	0.53	
1:E:169:SER:OG	1:E:172:VAL:HG23	2.08	0.53	
1:F:56:ASP:OD1	1:F:60:LYS:NZ	2.42	0.53	
1:H:56:ASP:OD1	1:H:60:LYS:NZ	2.42	0.53	
1:H:12:VAL:O	1:H:15:VAL:HG12	2.09	0.52	
1:E:144:TYR:OH	1:E:152:HIS:ND1	2.35	0.52	
1:C:39:LEU:HD13	1:C:120:LEU:HD23	1.91	0.52	
1:C:49:VAL:HG21	1:C:167:LEU:HD23	1.92	0.52	
1:A:162:VAL:HG11	1:C:49:VAL:HA	1.92	0.52	
1:B:95:ASP:O	1:B:216:PRO:HG3	2.11	0.51	
1:C:56:ASP:OD1	1:C:60:LYS:NZ	2.42	0.51	
1:H:60:LYS:HE2	1:H:112:ARG:HG2	1.91	0.51	
1:A:9:ASN:HB2	1:A:179:MET:HE1	1.92	0.51	
1:A:46:LEU:HD13	1:A:173:PHE:CE1	2.46	0.50	
1:G:39:LEU:HD13	1:G:120:LEU:HD23	1.91	0.50	
1:C:95:ASP:O	1:C:216:PRO:HG3	2.11	0.50	
1:H:67:LEU:HD22	1:H:76:TYR:CZ	2.47	0.50	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:99:HIS:CG	1:B:100:PRO:HD2	2.47	0.49	
1:A:96:HIS:O	3:A:438:HOH:O	2.20	0.49	
1:E:179:MET:HB3	1:E:184:GLN:OE1	2.12	0.49	
1:G:185:ALA:O	1:G:189:LEU:HG	2.11	0.49	
1:E:126:GLY:O	1:E:130:SER:HB3	2.12	0.49	
1:B:49:VAL:HA	1:E:162:VAL:HG11	1.94	0.49	
1:G:158:GLN:O	1:G:162:VAL:HG23	2.13	0.49	
1:H:54:SER:OG	3:H:410:HOH:O	2.20	0.48	
1:B:14:LEU:HD21	1:B:39:LEU:HD21	1.95	0.48	
1:B:155:ILE:HD12	1:E:52:PHE:HB2	1.96	0.47	
1:F:52:PHE:CE2	1:F:53:ILE:HG13	2.49	0.47	
1:H:144:TYR:OH	1:H:152:HIS:ND1	2.40	0.47	
1:G:51:SER:O	1:G:55:LYS:HG3	2.14	0.47	
1:B:154:TRP:CZ2	1:E:55:LYS:HB2	2.50	0.47	
1:B:154:TRP:HA	1:B:157:ARG:NH2	2.30	0.47	
1:F:95:ASP:O	1:F:216:PRO:HG3	2.15	0.47	
1:F:96:HIS:HA	3:F:409:HOH:O	2.14	0.47	
1:G:171:LYS:NZ	1:G:182:THR:HG21	2.30	0.47	
1:B:39:LEU:HD13	1:B:120:LEU:HD23	1.95	0.47	
1:G:46:LEU:HD13	1:G:173:PHE:CZ	2.50	0.47	
1:B:12:VAL:O	1:B:15:VAL:HG12	2.15	0.47	
1:B:154:TRP:HZ2	1:E:55:LYS:HB2	1.79	0.46	
1:B:212:LEU:HD22	1:B:215:LEU:HD11	1.96	0.46	
1:B:144:TYR:CZ	1:B:160:VAL:HG11	2.51	0.46	
1:B:185:ALA:O	1:B:189:LEU:HG	2.15	0.46	
1:A:177:MET:O	1:A:179:MET:HE2	2.15	0.46	
1:D:52:PHE:CE2	1:D:53:ILE:HG13	2.51	0.46	
1:H:212:LEU:O	1:H:215:LEU:HG	2.15	0.46	
1:A:57:VAL:O	1:A:61:LEU:HG	2.16	0.46	
1:H:51:SER:HB2	1:H:55:LYS:HE2	1.97	0.46	
1:D:147:THR:OG1	1:D:148:LEU:N	2.48	0.46	
1:H:10:LEU:O	1:H:14:LEU:HG	2.15	0.45	
1:C:136:THR:HG21	1:C:173:PHE:CE2	2.51	0.45	
1:A:120:LEU:HD12	1:A:120:LEU:HA	1.70	0.45	
1:C:111:LEU:HD21	1:C:115:ARG:NH2	2.31	0.45	
1:B:57:VAL:O	1:B:61:LEU:HG	2.16	0.45	
1:C:185:ALA:O	1:C:189:LEU:HG	2.16	0.45	
1:H:158:GLN:O	1:H:162:VAL:HG23	2.17	0.45	
1:A:209:GLU:HG2	1:B:45:SER:O	2.17	0.45	
1:F:108:ARG:NH2	1:F:216:PRO:OXT	2.41	0.45	
1:D:83:VAL:HG21	1:D:206:LEU:HD21	1.98	0.44	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:E:101:ARG:HE	1:E:101:ARG:HB3	1.42	0.44	
1:C:12:VAL:O	1:C:15:VAL:HG12	2.17	0.44	
1:A:155:ILE:HD12	1:C:52:PHE:HB2	1.98	0.44	
1:H:51:SER:HA	1:H:54:SER:HB3	1.99	0.44	
1:B:52:PHE:CE2	1:B:53:ILE:HG13	2.53	0.44	
1:B:60:LYS:HE2	1:B:112:ARG:HG2	2.00	0.43	
1:B:111:LEU:HD21	1:B:115:ARG:NH2	2.34	0.43	
1:F:120:LEU:HD12	1:F:120:LEU:HA	1.82	0.43	
1:F:119:TRP:CZ3	1:F:120:LEU:HD13	2.53	0.43	
1:G:169:SER:OG	1:G:172:VAL:HG23	2.18	0.43	
1:A:52:PHE:CE2	1:A:53:ILE:HG13	2.54	0.43	
1:C:158:GLN:O	1:C:162:VAL:HG23	2.19	0.43	
1:D:212:LEU:HD22	1:D:215:LEU:HD11	2.01	0.43	
1:F:144:TYR:CE2	1:F:149:ALA:HB2	2.54	0.43	
1:A:114:HIS:CE1	1:A:200:TYR:CE1	3.07	0.42	
1:C:136:THR:HG21	1:C:173:PHE:HE2	1.84	0.42	
1:D:120:LEU:HD12	1:D:120:LEU:HA	1.74	0.42	
1:F:154:TRP:O	1:F:158:GLN:HG2	2.18	0.42	
1:A:74:GLU:HG3	3:A:440:HOH:O	2.18	0.42	
1:D:152:HIS:O	1:D:157:ARG:NH2	2.52	0.42	
1:H:60:LYS:HA	1:H:63:ILE:HD12	2.00	0.42	
1:C:8:PHE:N	3:C:432:HOH:O	2.52	0.42	
1:F:51:SER:HB2	1:F:55:LYS:HE2	2.02	0.42	
1:H:124:LEU:HD23	1:H:124:LEU:HA	1.86	0.42	
1:B:52:PHE:HD2	1:E:155:ILE:HD11	1.84	0.42	
1:D:10:LEU:HA	1:D:10:LEU:HD12	1.82	0.42	
1:E:148:LEU:HA	1:E:148:LEU:HD23	1.84	0.42	
1:B:13:VAL:HG13	1:B:38:GLY:HA3	2.02	0.42	
1:D:36:TRP:HB3	1:D:61:LEU:HD11	2.02	0.42	
1:G:120:LEU:HD12	1:G:120:LEU:HA	1.80	0.42	
1:D:49:VAL:HG11	1:D:167:LEU:HD23	2.00	0.42	
1:A:51:SER:HB2	1:A:55:LYS:HE2	2.01	0.42	
1:A:56:ASP:OD1	1:A:60:LYS:NZ	2.45	0.42	
1:E:111:LEU:HB2	1:E:207:TYR:CE2	2.54	0.42	
1:H:108:ARG:NH1	2:H:301:PO4:O2	2.45	0.42	
1:C:114:HIS:ND1	3:C:416:HOH:O	2.36	0.42	
1:G:179:MET:HB3	1:G:184:GLN:OE1	2.19	0.41	
1:C:20:CYS:HB3	1:C:31:HIS:HB2	2.01	0.41	
1:E:56:ASP:OD1	1:E:60:LYS:NZ	2.52	0.41	
1:F:18:LYS:HD2	1:F:195:PHE:CZ	2.55	0.41	
1:E:108:ARG:HD3	1:E:108:ARG:C	2.41	0.41	



A 4 amo 1	A + 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:G:167:LEU:HA	1:G:168:PRO:HD3	1.79	0.41
1:A:114:HIS:CE1	1:A:200:TYR:CD1	3.08	0.41
1:B:174:LEU:HD23	1:B:174:LEU:HA	1.72	0.41
1:F:171:LYS:HD3	1:F:171:LYS:HA	1.87	0.41
1:B:162:VAL:CG1	1:E:49:VAL:HA	2.51	0.41
1:G:127:LEU:HD21	1:G:173:PHE:HB3	2.01	0.41
1:H:51:SER:HB2	1:H:55:LYS:NZ	2.36	0.41
1:F:51:SER:O	1:F:55:LYS:HG3	2.21	0.41
1:H:51:SER:HB2	1:H:55:LYS:CE	2.51	0.41
1:H:119:TRP:CZ3	1:H:120:LEU:HD13	2.56	0.41
1:C:154:TRP:CZ2	1:C:158:GLN:HG3	2.56	0.41
1:H:169:SER:OG	1:H:172:VAL:HG23	2.21	0.41
1:D:215:LEU:HA	1:D:216:PRO:HD2	1.85	0.41
1:E:20:CYS:SG	1:E:27:VAL:HG13	2.60	0.41
1:B:167:LEU:HA	1:B:168:PRO:HD3	1.89	0.40
1:C:127:LEU:HD21	1:C:173:PHE:HB3	2.02	0.40
1:E:120:LEU:HD12	1:E:120:LEU:HA	1.81	0.40
1:F:107:CYS:O	1:F:207:TYR:OH	2.32	0.40
1:G:60:LYS:HE2	1:G:112:ARG:HG2	2.02	0.40
1:H:51:SER:O	1:H:55:LYS:HG3	2.21	0.40
1:A:60:LYS:HE2	1:A:112:ARG:HG2	2.03	0.40
1:B:127:LEU:HA	1:B:127:LEU:HD12	1.92	0.40
1:D:131:SER:OG	1:D:131:SER:O	2.29	0.40
1:E:124:LEU:HD23	1:E:124:LEU:HA	1.87	0.40
1:E:111:LEU:HB2	1:E:207:TYR:HE2	1.86	0.40
1:E:193:LEU:HD23	1:E:193:LEU:HA	1.81	0.40
1:G:10:LEU:O	1:G:14:LEU:HG	2.22	0.40
1:G:212:LEU:HD22	1:G:215:LEU:HD11	2.03	0.40
1:H:51:SER:HB2	1:H:55:LYS:HZ3	1.87	0.40
1:B:10:LEU:HB3	1:B:188:MET:CE	2.52	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	202/217~(93%)	198~(98%)	4(2%)	0	100 100
1	В	203/217~(94%)	199~(98%)	4(2%)	0	100 100
1	С	201/217~(93%)	198 (98%)	3~(2%)	0	100 100
1	D	196/217~(90%)	194 (99%)	2(1%)	0	100 100
1	Е	203/217~(94%)	200 (98%)	3~(2%)	0	100 100
1	F	196/217~(90%)	192 (98%)	3~(2%)	1 (0%)	29 40
1	G	199/217~(92%)	196 (98%)	3~(2%)	0	100 100
1	Н	197/217~(91%)	194 (98%)	3 (2%)	0	100 100
All	All	1597/1736~(92%)	1571 (98%)	25~(2%)	1 (0%)	51 65

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	F	131	SER

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	Percentiles
1	А	178/194~(92%)	175~(98%)	3~(2%)	60 75
1	В	175/194~(90%)	170 (97%)	5(3%)	42 57
1	С	180/194~(93%)	176~(98%)	4 (2%)	52 66
1	D	178/194~(92%)	175~(98%)	3 (2%)	60 75
1	Ε	184/194~(95%)	180 (98%)	4 (2%)	52 66
1	F	174/194~(90%)	170~(98%)	4 (2%)	50 65
1	G	179/194~(92%)	176~(98%)	3~(2%)	60 75
1	Н	167/194~(86%)	164 (98%)	3 (2%)	59 74
All	All	1415/1552~(91%)	1386 (98%)	29 (2%)	55 70



\mathbf{Mol}	Chain	\mathbf{Res}	Type
1	А	77	THR
1	А	108	ARG
1	А	135	ARG
1	В	49	VAL
1	В	77	THR
1	В	92	VAL
1	В	108	ARG
1	В	173	PHE
1	С	77	THR
1	С	104	HIS
1	С	108	ARG
1	С	135	ARG
1	D	77	THR
1	D	108	ARG
1	D	173	PHE
1	Е	77	THR
1	Е	92	VAL
1	Е	108	ARG
1	Е	173	PHE
1	F	77	THR
1	F	104	HIS
1	F	108	ARG
1	F	173	PHE
1	G	77	THR
1	G	108	ARG
1	G	135	ARG
1	Н	77	THR
1	Н	108	ARG
1	Н	173	PHE

All (29) residues with a non-rotameric sidechain are listed below:

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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



5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	al Tuna Chain Pag Link		B	Bond lengths			Bond angles			
Moi Type	Type	Unain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	PO4	G	301	-	4,4,4	0.81	0	$6,\!6,\!6$	0.69	0
2	PO4	D	301	-	4,4,4	1.01	0	$6,\!6,\!6$	0.60	0
2	PO4	А	301	-	4,4,4	0.91	0	6,6,6	0.47	0
2	PO4	Н	301	-	4,4,4	0.89	0	6,6,6	0.48	0
2	PO4	В	301	-	4,4,4	0.96	0	6,6,6	0.66	0
2	PO4	Е	301	-	4,4,4	0.90	0	6,6,6	0.42	0
2	PO4	F	301	-	4,4,4	0.92	0	6,6,6	0.42	0
2	PO4	С	301	-	4,4,4	1.04	0	6,6,6	0.44	0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Н	301	PO4	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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	< RSRZ >	#RSRZ>2	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q < 0.9
1	А	206/217~(94%)	-0.24	0 100 100	29, 42, 64, 86	0
1	В	207/217~(95%)	-0.14	3 (1%) 75 81	29, 48, 79, 103	0
1	С	205/217~(94%)	-0.17	0 100 100	32, 42, 71, 98	0
1	D	202/217~(93%)	0.14	7 (3%) 44 51	32, 54, 98, 123	0
1	Е	207/217~(95%)	-0.06	2 (0%) 82 86	31, 49, 76, 109	0
1	F	202/217~(93%)	0.45	18 (8%) 9 11	34, 68, 109, 132	0
1	G	203/217~(93%)	-0.03	3 (1%) 73 79	33, 56, 81, 102	0
1	Н	203/217~(93%)	0.25	14 (6%) 16 20	36, 58, 104, 122	0
All	All	1635/1736~(94%)	0.02	47 (2%) 51 59	29, 51, 96, 132	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	173	PHE	7.1
1	F	155	ILE	6.5
1	F	156	VAL	4.4
1	F	162	VAL	4.3
1	F	52	PHE	4.1
1	Н	52	PHE	3.7
1	D	183	GLU	3.6
1	F	159	ALA	3.5
1	G	76	TYR	3.3
1	F	148	LEU	3.3
1	F	172	VAL	3.2
1	F	152	HIS	3.1
1	F	76	TYR	3.0
1	F	153	SER	3.0
1	Н	169	SER	3.0
1	В	96	HIS	2.9



Mol	Chain	Res	Type	RSRZ
1	Е	173	PHE	2.8
1	В	136	THR	2.8
1	D	169	SER	2.8
1	Н	76	TYR	2.7
1	В	167	LEU	2.7
1	Н	49	VAL	2.7
1	D	156	VAL	2.7
1	D	76	TYR	2.7
1	G	52	PHE	2.6
1	F	160	VAL	2.6
1	F	71	PRO	2.6
1	Н	72	GLN	2.5
1	Н	176	ALA	2.5
1	Н	172	VAL	2.5
1	D	182	THR	2.5
1	F	164	PHE	2.5
1	Н	173	PHE	2.5
1	F	127	LEU	2.4
1	D	8	PHE	2.4
1	Н	174	LEU	2.4
1	Е	159	ALA	2.4
1	Н	47	GLY	2.3
1	Н	155	ILE	2.3
1	F	49	VAL	2.3
1	F	53	ILE	2.3
1	D	195	PHE	2.2
1	Н	182	THR	2.2
1	F	94	MET	2.1
1	G	156	VAL	2.0
1	Н	46	LEU	2.0
1	Н	50	PHE	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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
2	PO4	F	301	5/5	0.87	0.19	80,90,99,105	0
2	PO4	Е	301	5/5	0.95	0.12	64,66,69,87	0
2	PO4	G	301	5/5	0.95	0.14	72,73,78,79	0
2	PO4	А	301	5/5	0.96	0.09	62,64,69,71	0
2	PO4	Н	301	5/5	0.96	0.14	82,83,87,88	0
2	PO4	С	301	5/5	0.98	0.13	$50,\!55,\!66,\!67$	0
2	PO4	D	301	5/5	0.98	0.10	67,69,79,81	0
2	PO4	В	301	5/5	0.98	0.11	47,51,60,62	0

6.5 Other polymers (i)

There are no such residues in this entry.

