Full wwPDB X-ray Structure Validation Report (i)

May 31, 2022 – 04:11 pm BST

PDB ID	:	7PGI
Title	:	NaVAb1p (bicelles)
Authors	:	Lolicato, M.; Arrigoni, C.
Deposited on	:	2021-08-14
Resolution	:	3.64 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 following versions of software and data (see references (1)) were used in the production of this report:

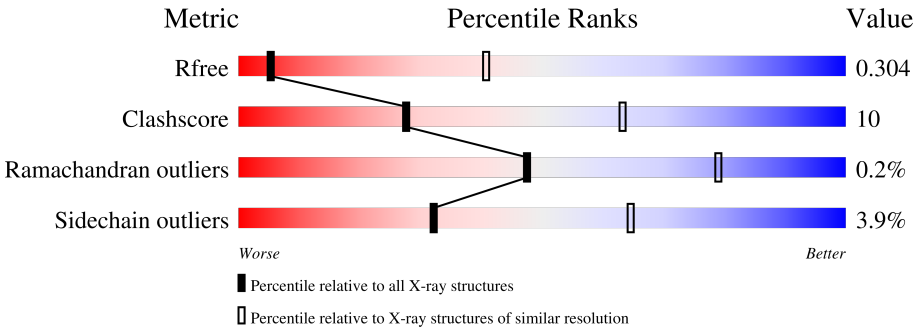
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.28.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.64 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}	130704	1341 (3.78-3.50)
Clashscore	141614	1439 (3.78-3.50)
Ramachandran outliers	138981	1391 (3.78-3.50)
Sidechain outliers	138945	1391 (3.78-3.50)

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%

Mol	Chain	Length	Quality of chain
1	A	150	75% 20%
1	B	150	75% 21%
1	C	150	75% 20%
1	D	150	77% 16% 5%
1	E	150	77% 19%
1	F	150	75% 19%
1	G	150	71% 24%

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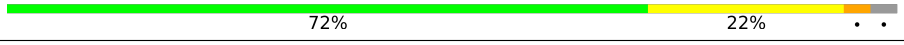
Mol	Chain	Length	Quality of chain
1	H	150	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9286 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 Ion transport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	146	Total	C	N	O	S	0	0	0
			1158	762	183	202	11			
1	B	146	Total	C	N	O	S	0	1	0
			1165	770	184	200	11			
1	C	146	Total	C	N	O	S	0	0	0
			1154	760	183	200	11			
1	D	147	Total	C	N	O	S	0	0	0
			1159	763	184	201	11			
1	E	147	Total	C	N	O	S	0	0	0
			1159	763	184	201	11			
1	F	146	Total	C	N	O	S	0	0	0
			1154	760	183	200	11			
1	G	146	Total	C	N	O	S	0	0	0
			1154	760	183	200	11			
1	H	146	Total	C	N	O	S	0	0	0
			1154	760	183	200	11			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ALA	deletion	UNP Q0VNY2
A	?	-	ALA	deletion	UNP Q0VNY2
B	?	-	ALA	deletion	UNP Q0VNY2
B	?	-	ALA	deletion	UNP Q0VNY2
C	?	-	ALA	deletion	UNP Q0VNY2
C	?	-	ALA	deletion	UNP Q0VNY2
D	?	-	ALA	deletion	UNP Q0VNY2
D	?	-	ALA	deletion	UNP Q0VNY2
E	?	-	ALA	deletion	UNP Q0VNY2
E	?	-	ALA	deletion	UNP Q0VNY2
F	?	-	ALA	deletion	UNP Q0VNY2
F	?	-	ALA	deletion	UNP Q0VNY2
G	?	-	ALA	deletion	UNP Q0VNY2

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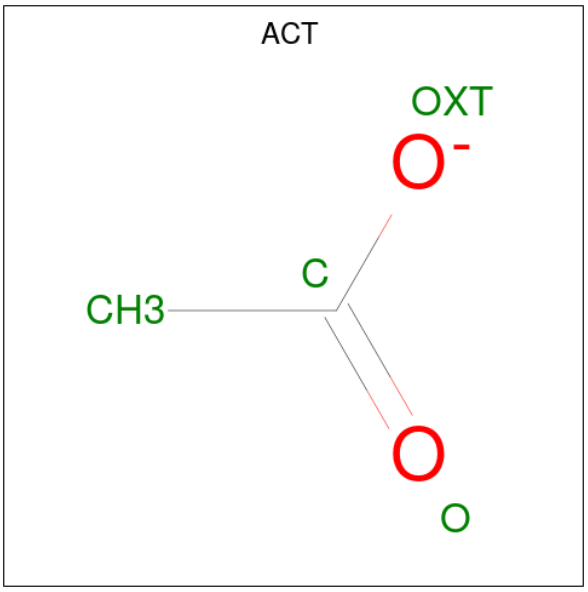
Chain	Residue	Modelled	Actual	Comment	Reference
G	?	-	ALA	deletion	UNP Q0VNY2
H	?	-	ALA	deletion	UNP Q0VNY2
H	?	-	ALA	deletion	UNP Q0VNY2

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Na 2 2	0	0
3	F	1	Total Na 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Na 1 1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

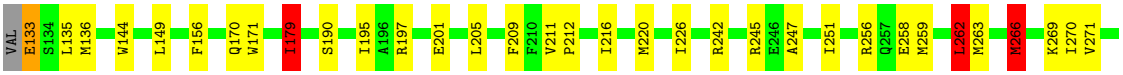
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total Mg 1 1	0	0

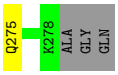
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: Ion transport protein

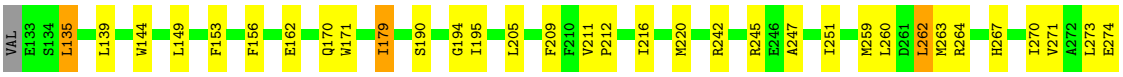
Chain A:

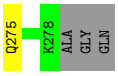




• Molecule 1: Ion transport protein

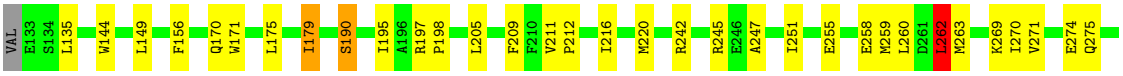
Chain B:





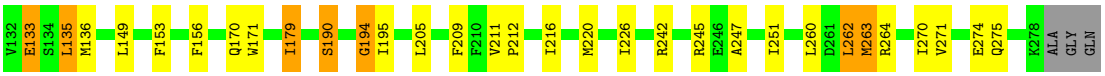
• Molecule 1: Ion transport protein

Chain C:



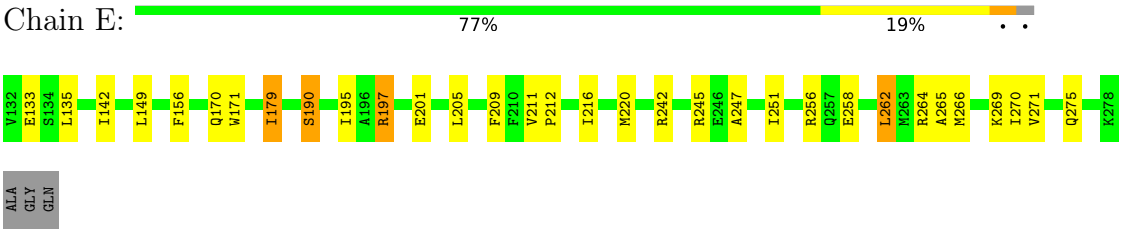
• Molecule 1: Ion transport protein

Chain D:



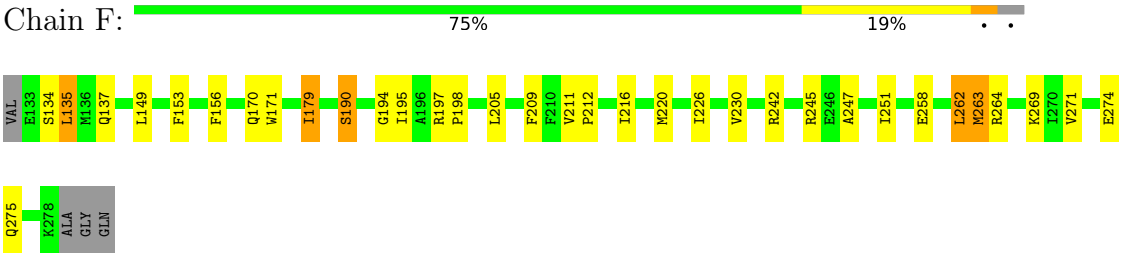
• Molecule 1: Ion transport protein

Chain E:



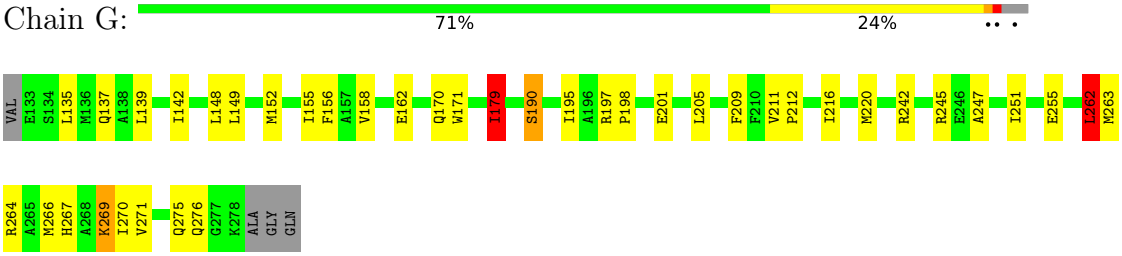
• Molecule 1: Ion transport protein

Chain F:



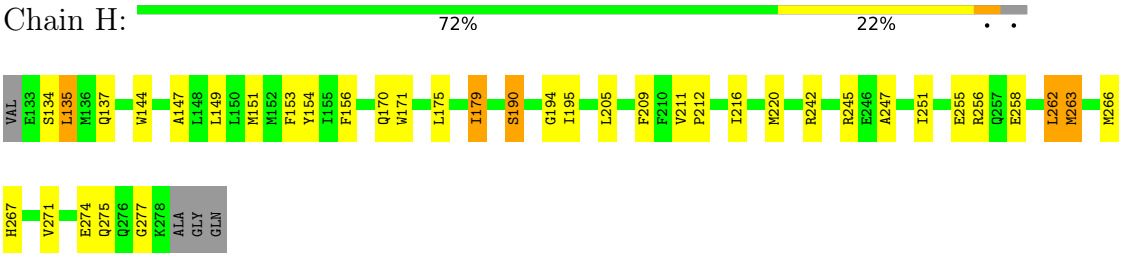
• Molecule 1: Ion transport protein

Chain G:



• Molecule 1: Ion transport protein

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	178.18Å 191.80Å 192.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.99 – 3.64 14.99 – 3.64	Depositor EDS
% Data completeness (in resolution range)	99.0 (14.99-3.64) 98.3 (14.99-3.64)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.20 (at 3.66Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.287 , 0.303 0.289 , 0.304	Depositor DCC
R_{free} test set	1755 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å^2)	129.2	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.20$	Xtriage
Estimated twinning fraction	0.250 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9286	wwPDB-VP
Average B, all atoms (Å^2)	130.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, NA, ACT

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	0.36	0/1187	0.69	6/1609 (0.4%)
1	B	0.32	0/1199	0.61	3/1627 (0.2%)
1	C	0.28	0/1183	0.57	3/1604 (0.2%)
1	D	0.27	0/1188	0.56	3/1611 (0.2%)
1	E	0.27	0/1188	0.59	3/1611 (0.2%)
1	F	0.27	0/1183	0.56	3/1604 (0.2%)
1	G	0.31	0/1183	0.60	3/1604 (0.2%)
1	H	0.28	0/1183	0.58	3/1604 (0.2%)
All	All	0.30	0/9494	0.60	27/12874 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	256	ARG	NE-CZ-NH2	7.96	124.28	120.30
1	G	262	LEU	CA-CB-CG	7.61	132.80	115.30
1	A	262	LEU	CA-CB-CG	7.58	132.73	115.30
1	C	262	LEU	CA-CB-CG	7.54	132.64	115.30
1	E	262	LEU	CA-CB-CG	7.53	132.63	115.30
1	A	266	MET	CB-CG-SD	-7.43	90.10	112.40
1	A	256	ARG	NE-CZ-NH1	-6.79	116.91	120.30
1	F	262	LEU	CA-CB-CG	6.17	129.50	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	179	ILE	CG1-CB-CG2	-6.14	97.88	111.40
1	C	179	ILE	CG1-CB-CG2	-6.11	97.96	111.40
1	D	262	LEU	CA-CB-CG	6.10	129.33	115.30
1	H	262	LEU	CA-CB-CG	6.09	129.32	115.30
1	A	179	ILE	CG1-CB-CG2	-6.06	98.07	111.40
1	G	179	ILE	CG1-CB-CG2	-6.05	98.09	111.40
1	B	135	LEU	CB-CG-CD2	-5.92	100.94	111.00
1	H	135	LEU	CA-CB-CG	5.80	128.65	115.30
1	B	262	LEU	CA-CB-CG	5.74	128.49	115.30
1	F	263	MET	CA-CB-CG	5.66	122.91	113.30
1	H	263	MET	CA-CB-CG	5.66	122.92	113.30
1	D	135	LEU	CA-CB-CG	5.62	128.22	115.30
1	B	135	LEU	CA-CB-CG	5.60	128.19	115.30
1	F	135	LEU	CA-CB-CG	5.53	128.03	115.30
1	C	262	LEU	CB-CG-CD2	-5.47	101.69	111.00
1	D	263	MET	CA-CB-CG	5.44	122.54	113.30
1	A	262	LEU	CB-CG-CD2	-5.36	101.89	111.00
1	E	262	LEU	CB-CG-CD2	-5.14	102.26	111.00
1	G	262	LEU	CB-CG-CD2	-5.02	102.46	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	133	GLU	Peptide

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	1158	0	1146	37	0
1	B	1165	0	1152	43	0
1	C	1154	0	1142	31	0
1	D	1159	0	1144	26	0
1	E	1159	0	1144	19	0
1	F	1154	0	1142	24	0
1	G	1154	0	1141	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1154	0	1142	31	0
2	A	4	0	3	0	0
2	C	4	0	3	0	0
2	D	4	0	3	0	0
2	E	4	0	3	0	0
2	G	4	0	3	0	0
2	H	4	0	3	0	0
3	A	2	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
4	E	1	0	0	0	0
All	All	9286	0	9171	184	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 10.

All (184) 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:C:263:MET:HG2	1:D:263:MET:HE1	1.37	1.04
1:A:266:MET:HE1	1:B:267:HIS:HD2	1.31	0.96
1:A:266:MET:HE1	1:B:267:HIS:CD2	2.06	0.91
1:A:133:GLU:N	1:A:133:GLU:OE2	2.08	0.87
1:A:266:MET:CE	1:B:267:HIS:HD2	1.95	0.80
1:A:266:MET:CE	1:B:270:ILE:HB	2.16	0.76
1:A:170:GLN:HG2	1:A:171:TRP:N	2.01	0.76
1:A:266:MET:HE3	1:B:270:ILE:CG2	2.16	0.75
1:A:266:MET:HE3	1:B:270:ILE:HB	1.69	0.74
1:A:266:MET:HE3	1:B:270:ILE:CB	2.19	0.73
1:A:263:MET:HG2	1:B:263:MET:HE3	1.71	0.72
1:A:266:MET:CE	1:B:267:HIS:CD2	2.73	0.71
1:A:197:ARG:O	1:A:201:GLU:HB2	1.94	0.67
1:C:259:MET:HG2	1:D:260:LEU:HG	1.80	0.64
1:H:170:GLN:HG2	1:H:171:TRP:N	2.13	0.64
1:B:190:SER:HB2	1:B:195:ILE:H	1.61	0.63
1:B:273:LEU:HD21	1:C:274:GLU:HB2	1.82	0.62
1:A:258:GLU:OE2	1:B:264:ARG:NH2	2.32	0.62
1:A:259:MET:HG2	1:B:260:LEU:HG	1.80	0.62
1:B:270:ILE:HD11	1:C:270:ILE:HD13	1.81	0.61
1:E:265:ALA:O	1:E:269:LYS:HG2	2.00	0.61
1:H:134:SER:O	1:H:137:GLN:HG2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:256:ARG:NE	1:H:255:GLU:OE1	2.24	0.60
1:A:263:MET:HG2	1:B:263:MET:CE	2.30	0.60
1:A:269:LYS:HE2	1:B:274:GLU:OE1	2.02	0.59
1:B:149:LEU:HD13	1:B:220:MET:HB2	1.85	0.59
1:G:262:LEU:HG	1:H:263:MET:HE2	1.85	0.59
1:F:190:SER:O	1:F:194:GLY:HA2	2.02	0.59
1:C:270:ILE:HD11	1:D:270:ILE:HD12	1.84	0.59
1:H:149:LEU:HD13	1:H:220:MET:HB2	1.85	0.59
1:C:149:LEU:HD13	1:C:220:MET:HB2	1.85	0.59
1:F:149:LEU:HD13	1:F:220:MET:HB2	1.85	0.59
1:A:149:LEU:HD13	1:A:220:MET:HB2	1.85	0.58
1:A:270:ILE:HD11	1:B:270:ILE:HD12	1.85	0.58
1:G:149:LEU:HD13	1:G:220:MET:HB2	1.85	0.58
1:G:197:ARG:HB2	1:G:198:PRO:HD3	1.86	0.58
1:E:149:LEU:HD13	1:E:220:MET:HB2	1.85	0.58
1:E:264:ARG:NH2	1:H:258:GLU:OE2	2.36	0.57
1:D:149:LEU:HD13	1:D:220:MET:HB2	1.85	0.57
1:G:276:GLN:HE22	1:H:277:GLY:HA2	1.69	0.57
1:A:266:MET:HE2	1:B:267:HIS:HA	1.87	0.57
1:G:162:GLU:HG3	1:H:175:LEU:HD23	1.86	0.57
1:A:171:TRP:CE3	1:A:195:ILE:HG23	2.39	0.57
1:C:263:MET:HG2	1:D:263:MET:CE	2.24	0.57
1:H:190:SER:HB2	1:H:195:ILE:H	1.70	0.56
1:H:190:SER:OG	1:H:190:SER:O	2.23	0.56
1:H:190:SER:O	1:H:194:GLY:HA2	2.06	0.56
1:F:190:SER:HB2	1:F:195:ILE:H	1.71	0.56
1:D:190:SER:O	1:D:194:GLY:HA2	2.06	0.55
1:F:230:VAL:HG21	1:G:137:GLN:HA	1.87	0.55
1:G:171:TRP:CE3	1:G:195:ILE:HG23	2.42	0.55
1:C:171:TRP:CE3	1:C:195:ILE:HG23	2.42	0.55
1:A:266:MET:HE2	1:B:270:ILE:HB	1.89	0.55
1:B:171:TRP:CE3	1:B:195:ILE:HG23	2.42	0.55
1:D:171:TRP:CE3	1:D:195:ILE:HG23	2.42	0.55
1:E:171:TRP:CE3	1:E:195:ILE:HG23	2.42	0.55
1:C:262:LEU:HD21	1:D:264:ARG:HG2	1.89	0.54
1:D:190:SER:HB2	1:D:195:ILE:H	1.72	0.54
1:H:171:TRP:CE3	1:H:195:ILE:HG23	2.42	0.54
1:F:171:TRP:CE3	1:F:195:ILE:HG23	2.42	0.54
1:E:197:ARG:O	1:E:201:GLU:HG3	2.08	0.54
1:C:170:GLN:HG2	1:C:171:TRP:N	2.22	0.53
1:B:270:ILE:CD1	1:C:270:ILE:HD13	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:216:ILE:O	1:E:220:MET:HG2	2.10	0.52
1:B:190:SER:O	1:B:194:GLY:HA2	2.08	0.52
1:C:190:SER:OG	1:C:190:SER:O	2.28	0.52
1:A:216:ILE:O	1:A:220:MET:HG2	2.10	0.52
1:F:134:SER:O	1:F:137:GLN:HG2	2.09	0.52
1:D:216:ILE:O	1:D:220:MET:HG2	2.10	0.52
1:F:216:ILE:O	1:F:220:MET:HG2	2.10	0.52
1:G:216:ILE:O	1:G:220:MET:HG2	2.10	0.52
1:H:216:ILE:O	1:H:220:MET:HG2	2.10	0.52
1:A:266:MET:HE3	1:B:270:ILE:HG21	1.90	0.52
1:C:216:ILE:O	1:C:220:MET:HG2	2.10	0.52
1:D:190:SER:O	1:D:190:SER:OG	2.25	0.51
1:F:226:ILE:HD13	1:G:139:LEU:HD12	1.91	0.51
1:B:259:MET:HG2	1:C:260:LEU:HG	1.92	0.51
1:B:216:ILE:O	1:B:220:MET:HG2	2.10	0.51
1:E:269:LYS:HE2	1:F:274:GLU:OE1	2.10	0.50
1:A:266:MET:O	1:A:266:MET:SD	2.70	0.49
1:B:170:GLN:HG2	1:B:171:TRP:N	2.27	0.49
1:B:144:TRP:HE3	1:C:144:TRP:CH2	2.31	0.49
1:F:190:SER:O	1:F:190:SER:OG	2.21	0.49
1:A:266:MET:CE	1:B:270:ILE:CB	2.84	0.48
1:B:271:VAL:O	1:B:275:GLN:HG3	2.13	0.48
1:D:156:PHE:HD1	1:D:209:PHE:CE1	2.32	0.48
1:D:170:GLN:HG2	1:D:171:TRP:N	2.29	0.48
1:C:270:ILE:HD11	1:D:270:ILE:CD1	2.43	0.48
1:E:170:GLN:HG2	1:E:171:TRP:N	2.29	0.48
1:C:271:VAL:O	1:C:275:GLN:HG3	2.14	0.48
1:B:263:MET:HG2	1:C:263:MET:HE3	1.95	0.47
1:B:156:PHE:HD1	1:B:209:PHE:CE1	2.31	0.47
1:B:211:VAL:HB	1:B:212:PRO:HD3	1.96	0.47
1:A:156:PHE:HD1	1:A:209:PHE:CE1	2.32	0.47
1:A:211:VAL:HB	1:A:212:PRO:HD3	1.97	0.47
1:G:266:MET:O	1:G:270:ILE:HG13	2.13	0.47
1:A:136:MET:SD	1:D:226:ILE:HG23	2.54	0.47
1:F:211:VAL:HB	1:F:212:PRO:HD3	1.97	0.47
1:F:258:GLU:OE2	1:G:264:ARG:NH2	2.46	0.47
1:B:270:ILE:HD11	1:C:270:ILE:CD1	2.44	0.47
1:F:156:PHE:HD1	1:F:209:PHE:CE1	2.32	0.47
1:G:170:GLN:HG2	1:G:171:TRP:N	2.29	0.47
1:H:211:VAL:HB	1:H:212:PRO:HD3	1.97	0.47
1:A:271:VAL:O	1:A:275:GLN:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:170:GLN:HG2	1:F:171:TRP:N	2.29	0.47
1:F:197:ARG:HB2	1:F:198:PRO:HD3	1.96	0.47
1:C:156:PHE:HD1	1:C:209:PHE:CE1	2.32	0.47
1:G:156:PHE:HD1	1:G:209:PHE:CE1	2.32	0.47
1:G:276:GLN:HE22	1:H:277:GLY:CA	2.28	0.47
1:H:156:PHE:HD1	1:H:209:PHE:CE1	2.32	0.47
1:E:266:MET:O	1:E:270:ILE:HG13	2.14	0.47
1:F:271:VAL:O	1:F:275:GLN:HG3	2.15	0.47
1:D:271:VAL:O	1:D:275:GLN:HG3	2.15	0.47
1:H:271:VAL:O	1:H:275:GLN:HG3	2.15	0.47
1:E:190:SER:O	1:E:190:SER:OG	2.26	0.46
1:D:211:VAL:HB	1:D:212:PRO:HD3	1.97	0.46
1:E:156:PHE:HD1	1:E:209:PHE:CE1	2.32	0.46
1:E:271:VAL:O	1:E:275:GLN:HG3	2.15	0.46
1:G:262:LEU:HD11	1:H:267:HIS:HB2	1.96	0.46
1:A:262:LEU:HD21	1:B:264:ARG:HG2	1.97	0.46
1:H:242:ARG:O	1:H:245:ARG:N	2.48	0.46
1:E:211:VAL:HB	1:E:212:PRO:HD3	1.97	0.46
1:D:242:ARG:O	1:D:245:ARG:N	2.48	0.46
1:E:242:ARG:O	1:E:245:ARG:N	2.49	0.46
1:G:158:VAL:HG11	1:H:154:TYR:OH	2.15	0.46
1:A:242:ARG:O	1:A:245:ARG:N	2.49	0.46
1:C:242:ARG:O	1:C:245:ARG:N	2.49	0.46
1:G:211:VAL:HB	1:G:212:PRO:HD3	1.97	0.46
1:B:242:ARG:O	1:B:245:ARG:N	2.48	0.46
1:G:267:HIS:O	1:G:271:VAL:HG23	2.16	0.46
1:G:190:SER:O	1:G:190:SER:OG	2.28	0.46
1:G:242:ARG:O	1:G:245:ARG:N	2.49	0.46
1:B:162:GLU:HG3	1:C:175:LEU:HB3	1.98	0.45
1:C:197:ARG:HB2	1:C:198:PRO:HD3	1.96	0.45
1:G:255:GLU:OE1	1:H:256:ARG:NE	2.37	0.45
1:G:271:VAL:O	1:G:275:GLN:HG3	2.16	0.45
1:E:258:GLU:OE2	1:F:264:ARG:NH2	2.48	0.45
1:C:211:VAL:HB	1:C:212:PRO:HD3	1.97	0.45
1:F:263:MET:HB3	1:F:263:MET:HE3	1.75	0.45
1:G:155:ILE:HD13	1:H:151:MET:SD	2.57	0.45
1:B:153:PHE:HB3	1:B:179:ILE:CD1	2.47	0.44
1:F:269:LYS:HE2	1:G:271:VAL:HG22	1.99	0.44
1:B:190:SER:O	1:B:190:SER:OG	2.32	0.44
1:H:153:PHE:HB3	1:H:179:ILE:CD1	2.48	0.44
1:F:242:ARG:O	1:F:245:ARG:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:MET:O	1:A:270:ILE:HG13	2.18	0.44
1:C:270:ILE:CD1	1:D:270:ILE:HD12	2.47	0.44
1:A:205:LEU:HD23	1:A:205:LEU:H	1.83	0.44
1:C:263:MET:HE2	1:C:263:MET:HB3	1.72	0.44
1:E:205:LEU:HD23	1:E:205:LEU:H	1.83	0.43
1:D:205:LEU:H	1:D:205:LEU:HD23	1.83	0.43
1:D:153:PHE:HB3	1:D:179:ILE:CD1	2.48	0.43
1:F:153:PHE:HB3	1:F:179:ILE:CD1	2.48	0.43
1:C:269:LYS:HE2	1:D:274:GLU:OE1	2.19	0.43
1:A:179:ILE:HD12	1:A:179:ILE:HA	1.84	0.43
1:C:205:LEU:H	1:C:205:LEU:HD23	1.83	0.43
1:H:205:LEU:H	1:H:205:LEU:HD23	1.83	0.43
1:F:205:LEU:H	1:F:205:LEU:HD23	1.84	0.43
1:B:205:LEU:HD23	1:B:205:LEU:H	1.83	0.43
1:E:247:ALA:O	1:E:251:ILE:HG12	2.19	0.43
1:G:205:LEU:H	1:G:205:LEU:HD23	1.83	0.42
1:D:179:ILE:HD13	1:D:179:ILE:HA	1.83	0.42
1:A:247:ALA:O	1:A:251:ILE:HG12	2.19	0.42
1:B:247:ALA:O	1:B:251:ILE:HG12	2.19	0.42
1:A:144:TRP:HE3	1:B:144:TRP:CH2	2.37	0.42
1:C:247:ALA:O	1:C:251:ILE:HG12	2.20	0.42
1:F:247:ALA:O	1:F:251:ILE:HG12	2.19	0.42
1:G:179:ILE:HD12	1:G:179:ILE:HA	1.84	0.42
1:G:263:MET:HG2	1:H:263:MET:HE1	2.02	0.42
1:G:269:LYS:HG3	1:H:274:GLU:OE1	2.20	0.42
1:H:247:ALA:O	1:H:251:ILE:HG12	2.20	0.42
1:G:197:ARG:O	1:G:201:GLU:HG3	2.20	0.42
1:D:247:ALA:O	1:D:251:ILE:HG12	2.20	0.41
1:G:148:LEU:HD12	1:H:144:TRP:CD1	2.55	0.41
1:E:197:ARG:HD3	1:E:197:ARG:H	1.85	0.41
1:G:152:MET:HE3	1:H:147:ALA:HB1	2.02	0.41
1:F:179:ILE:HD13	1:F:179:ILE:HA	1.83	0.41
1:G:247:ALA:O	1:G:251:ILE:HG12	2.19	0.41
1:G:266:MET:HE1	1:H:266:MET:HB3	2.03	0.41
1:A:226:ILE:HD13	1:B:139:LEU:HD12	2.02	0.41
1:C:258:GLU:OE2	1:D:264:ARG:NH2	2.46	0.41
1:C:255:GLU:O	1:C:259:MET:HG3	2.21	0.40
1:D:133:GLU:HA	1:D:136:MET:HB3	2.04	0.40
1:H:179:ILE:HD13	1:H:179:ILE:HA	1.83	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	Percentiles	
1	A	144/150 (96%)	139 (96%)	5 (4%)	0	100	100
1	B	145/150 (97%)	143 (99%)	2 (1%)	0	100	100
1	C	144/150 (96%)	141 (98%)	3 (2%)	0	100	100
1	D	145/150 (97%)	141 (97%)	3 (2%)	1 (1%)	22	61
1	E	145/150 (97%)	141 (97%)	3 (2%)	1 (1%)	22	61
1	F	144/150 (96%)	140 (97%)	4 (3%)	0	100	100
1	G	144/150 (96%)	142 (99%)	2 (1%)	0	100	100
1	H	144/150 (96%)	141 (98%)	3 (2%)	0	100	100
All	All	1155/1200 (96%)	1128 (98%)	25 (2%)	2 (0%)	47	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	133	GLU
1	D	194	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	119/124 (96%)	113 (95%)	6 (5%)	24	58
1	B	119/124 (96%)	116 (98%)	3 (2%)	47	74
1	C	118/124 (95%)	114 (97%)	4 (3%)	37	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	118/124 (95%)	114 (97%)	4 (3%)	37 68
1	E	118/124 (95%)	112 (95%)	6 (5%)	24 58
1	F	118/124 (95%)	114 (97%)	4 (3%)	37 68
1	G	118/124 (95%)	112 (95%)	6 (5%)	24 58
1	H	118/124 (95%)	114 (97%)	4 (3%)	37 68
All	All	946/992 (95%)	909 (96%)	37 (4%)	32 64

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	GLU
1	A	135	LEU
1	A	179	ILE
1	A	190	SER
1	A	262	LEU
1	A	266	MET
1	B	135	LEU
1	B	179	ILE
1	B	262	LEU
1	C	135	LEU
1	C	179	ILE
1	C	190	SER
1	C	262	LEU
1	D	135	LEU
1	D	179	ILE
1	D	190	SER
1	D	262	LEU
1	E	135	LEU
1	E	142	ILE
1	E	179	ILE
1	E	190	SER
1	E	197	ARG
1	E	262	LEU
1	F	135	LEU
1	F	179	ILE
1	F	190	SER
1	F	262	LEU
1	G	135	LEU
1	G	142	ILE
1	G	179	ILE

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Mol	Chain	Res	Type
1	G	190	SER
1	G	262	LEU
1	G	269	LYS
1	H	135	LEU
1	H	179	ILE
1	H	190	SER
1	H	262	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	267	HIS
1	G	276	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ACT	C	301	3	1,3,3	6.74	1 (100%)	0,3,3	-	-
2	ACT	G	302	-	1,3,3	6.22	1 (100%)	0,3,3	-	-
2	ACT	D	401	3	1,3,3	6.60	1 (100%)	0,3,3	-	-
2	ACT	E	302	3	1,3,3	6.39	1 (100%)	0,3,3	-	-
2	ACT	H	401	-	1,3,3	6.50	1 (100%)	0,3,3	-	-
2	ACT	A	501	3	1,3,3	6.55	1 (100%)	0,3,3	-	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	ACT	CH3-C	6.74	1.57	1.48
2	D	401	ACT	CH3-C	6.60	1.57	1.48
2	A	501	ACT	CH3-C	6.55	1.57	1.48
2	H	401	ACT	CH3-C	6.50	1.57	1.48
2	E	302	ACT	CH3-C	6.39	1.56	1.48
2	G	302	ACT	CH3-C	6.22	1.56	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.