



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 10:10 am BST

PDB ID : 6BAQ
Title : Mus musculus BPIFA1
Authors : Little, M.S.; Redinbo, M.R.
Deposited on : 2017-10-15
Resolution : 2.50 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

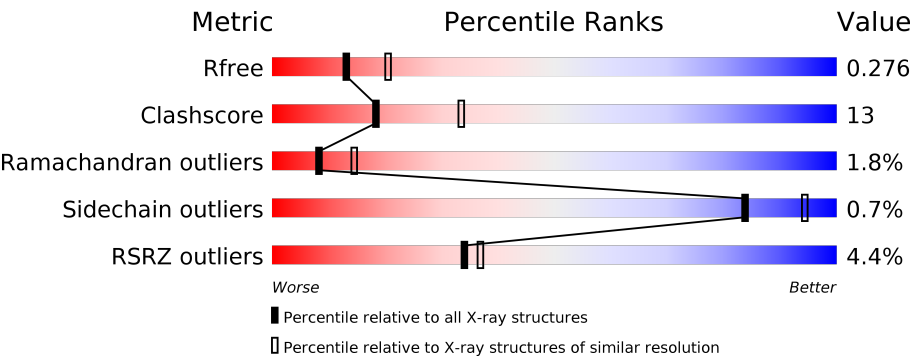
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 on 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 $\leq 5\%$. 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	244	<div><div>2%</div><div><div></div><div>64%</div><div>15%</div><div>•</div><div>20%</div></div></div>
1	B	244	<div><div>3%</div><div><div></div><div>59%</div><div>18%</div><div>•</div><div>21%</div></div></div>
1	C	244	<div><div>5%</div><div><div></div><div>53%</div><div>23%</div><div>•</div><div>23%</div></div></div>
1	D	244	<div><div>4%</div><div><div></div><div>59%</div><div>17%</div><div>•</div><div>22%</div></div></div>
1	E	244	<div><div>4%</div><div><div></div><div>61%</div><div>18%</div><div>•</div><div>20%</div></div></div>
1	F	244	<div><div>2%</div><div><div></div><div>71%</div><div>14%</div><div>•</div><div>14%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	244	
1	H	244	

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
2	NA	D	304	-	-	-	X
2	NA	G	313	-	-	-	X
3	CL	B	307	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11502 atoms, of which 32 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 BPI fold-containing family A member 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	196	Total	C	N	O	S	0	0	0
			1400	909	228	260	3			
1	B	192	Total	C	N	O	S	0	1	0
			1360	878	225	254	3			
1	C	187	Total	C	N	O	S	0	0	0
			1329	861	217	248	3			
1	D	190	Total	C	N	O	S	0	0	0
			1335	866	220	246	3			
1	E	196	Total	C	N	O	S	0	0	0
			1394	897	231	263	3			
1	F	211	Total	C	N	O	S	0	0	0
			1501	972	246	280	3			
1	G	195	Total	C	N	O	S	0	0	0
			1380	886	230	261	3			
1	H	191	Total	C	N	O	S	0	0	0
			1358	880	221	254	3			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	SER	-	expression tag	UNP P97361
A	36	ASN	-	expression tag	UNP P97361
A	37	ALA	-	expression tag	UNP P97361
B	35	SER	-	expression tag	UNP P97361
B	36	ASN	-	expression tag	UNP P97361
B	37	ALA	-	expression tag	UNP P97361
C	35	SER	-	expression tag	UNP P97361
C	36	ASN	-	expression tag	UNP P97361
C	37	ALA	-	expression tag	UNP P97361
D	35	SER	-	expression tag	UNP P97361
D	36	ASN	-	expression tag	UNP P97361
D	37	ALA	-	expression tag	UNP P97361
E	35	SER	-	expression tag	UNP P97361

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Chain	Residue	Modelled	Actual	Comment	Reference
E	36	ASN	-	expression tag	UNP P97361
E	37	ALA	-	expression tag	UNP P97361
F	35	SER	-	expression tag	UNP P97361
F	36	ASN	-	expression tag	UNP P97361
F	37	ALA	-	expression tag	UNP P97361
G	35	SER	-	expression tag	UNP P97361
G	36	ASN	-	expression tag	UNP P97361
G	37	ALA	-	expression tag	UNP P97361
H	35	SER	-	expression tag	UNP P97361
H	36	ASN	-	expression tag	UNP P97361
H	37	ALA	-	expression tag	UNP P97361

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	13	Total 13	Na 13	0	0
2	D	4	Total 4	Na 4	0	0
2	E	9	Total 9	Na 9	0	0
2	H	7	Total 7	Na 7	0	0
2	B	6	Total 6	Na 6	0	0
2	C	8	Total 8	Na 8	0	0
2	A	11	Total 11	Na 11	0	0
2	F	5	Total 5	Na 5	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Cl 1	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	H	O	0	0
			14	3	8	3		
4	G	1	Total	C	H	O	0	0
			14	3	8	3		
4	H	1	Total	C	H	O	0	0
			14	3	8	3		
4	H	1	Total	C	H	O	0	0
			14	3	8	3		

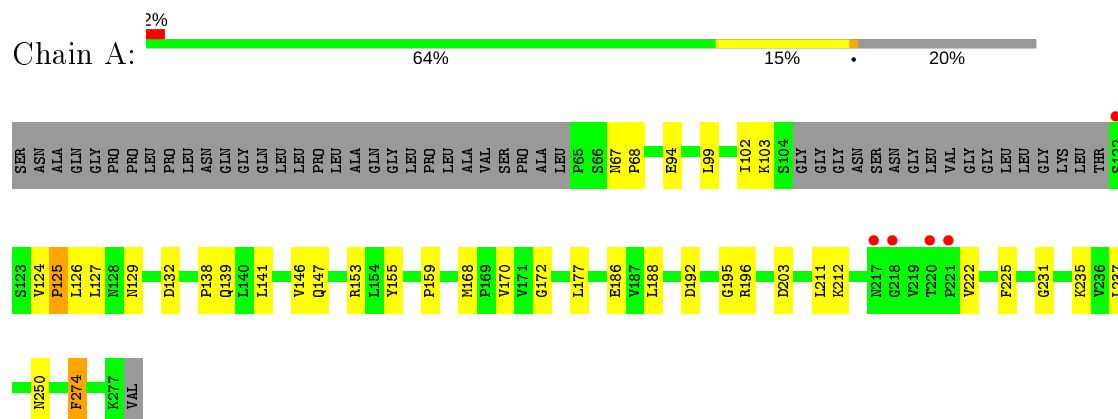
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	74	Total	O	0	0
			74	74		
5	B	21	Total	O	0	0
			21	21		
5	C	17	Total	O	0	0
			17	17		
5	D	27	Total	O	0	0
			27	27		
5	E	53	Total	O	0	0
			53	53		
5	F	74	Total	O	0	0
			74	74		
5	G	41	Total	O	0	0
			41	41		
5	H	18	Total	O	0	0
			18	18		

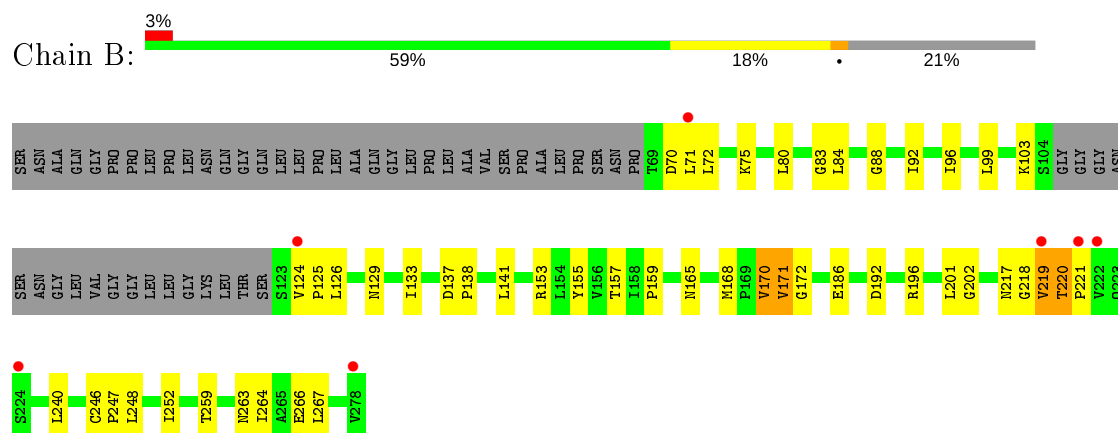
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

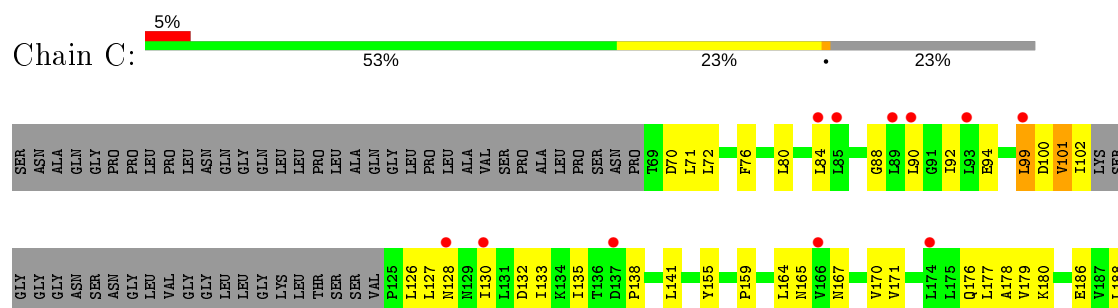
- Molecule 1: BPI fold-containing family A member 1



- Molecule 1: BPI fold-containing family A member 1

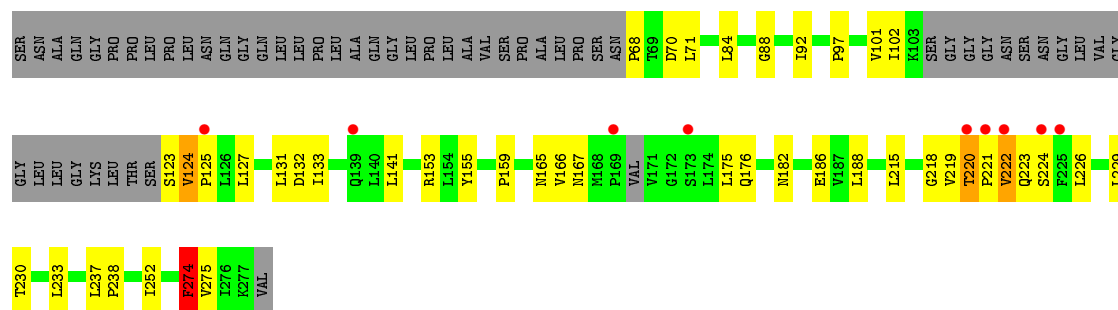


- Molecule 1: BPI fold-containing family A member 1

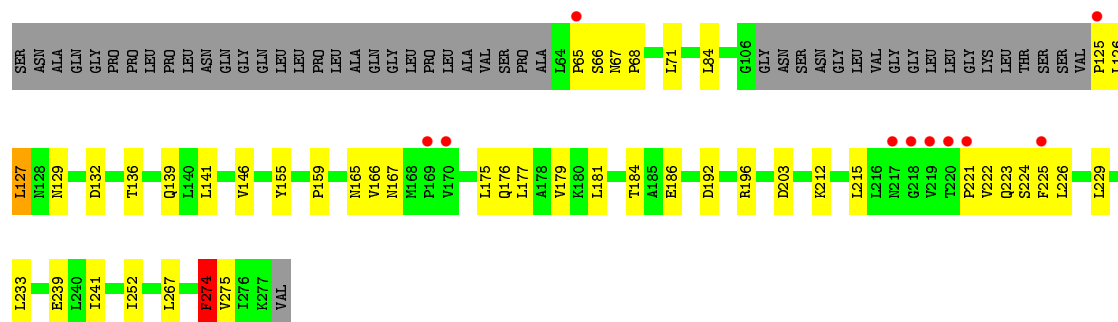




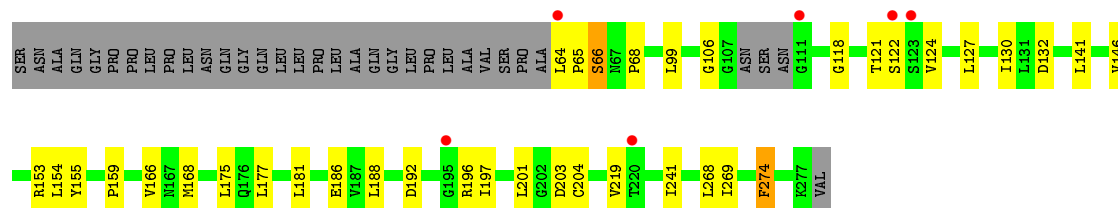
- Molecule 1: BPI fold-containing family A member 1



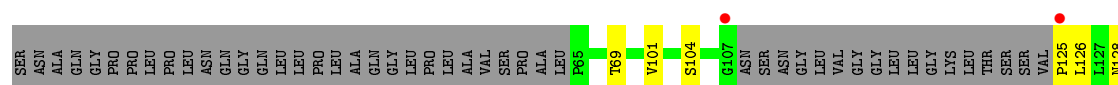
- Molecule 1: BPI fold-containing family A member 1

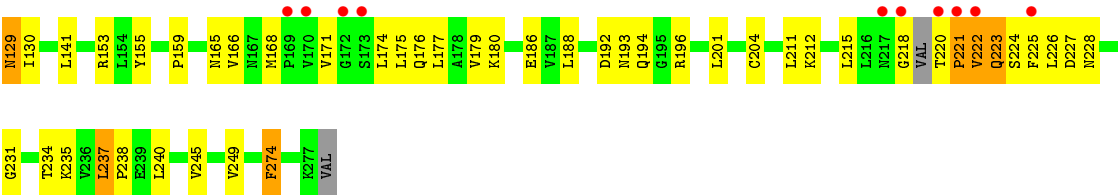


- Molecule 1: BPI fold-containing family A member 1

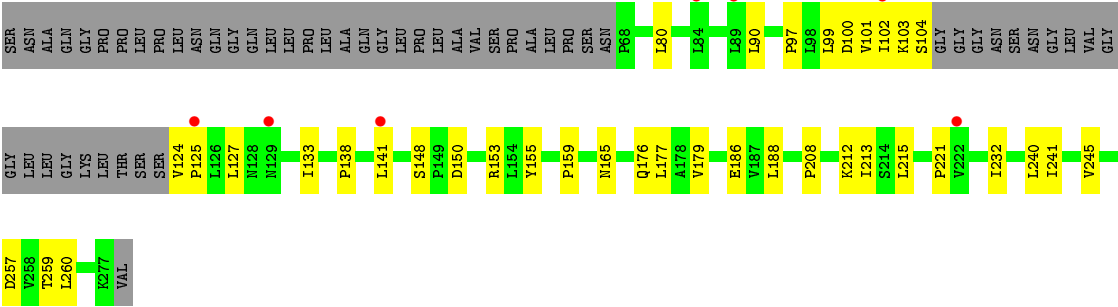


- Molecule 1: BPI fold-containing family A member 1





• Molecule 1: BPI fold-containing family A member 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	132.20Å 200.58Å 89.50Å 90.00° 126.15° 90.00°	Depositor
Resolution (Å)	41.79 – 2.50 44.49 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.8 (41.79-2.50) 94.5 (44.49-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.39 (at 2.51Å)	Xtriage
Refinement program	Coot 1.12_2829, PHENIX 1.12_2829	Depositor
R, R_{free}	0.221 , 0.278 0.224 , 0.276	Depositor DCC
R_{free} test set	1992 reflections (3.10%)	wwPDB-VP
Wilson B-factor (Å ²)	30.5	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 66.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11502	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 72.50 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.1779e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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.

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, CL, NA

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	0.42	0/1419	0.69	1/1944 (0.1%)
1	B	0.40	0/1377	0.67	0/1886
1	C	0.38	0/1346	0.65	0/1845
1	D	0.41	0/1352	0.68	1/1852 (0.1%)
1	E	0.42	0/1412	0.71	2/1931 (0.1%)
1	F	0.43	0/1520	0.69	0/2079
1	G	0.42	0/1398	0.65	1/1909 (0.1%)
1	H	0.37	0/1376	0.61	0/1887
All	All	0.41	0/11200	0.67	5/15333 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	274	PHE	CB-CG-CD2	-7.31	115.68	120.80
1	D	274	PHE	CB-CG-CD2	-6.44	116.29	120.80
1	G	237	LEU	CA-CB-CG	5.79	128.61	115.30
1	E	274	PHE	CB-CG-CD1	5.45	124.62	120.80
1	A	237	LEU	CA-CB-CG	5.36	127.62	115.30

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	1400	0	1446	37	0
1	B	1360	0	1365	38	0
1	C	1329	0	1358	52	0
1	D	1335	0	1350	38	0
1	E	1394	0	1420	42	0
1	F	1501	0	1570	31	0
1	G	1380	0	1400	41	0
1	H	1358	0	1386	31	0
2	A	11	0	0	0	0
2	B	6	0	0	0	0
2	C	8	0	0	0	0
2	D	4	0	0	0	0
2	E	9	0	0	0	0
2	F	5	0	0	0	0
2	G	13	0	0	0	0
2	H	7	0	0	0	0
3	B	1	0	0	2	0
4	C	6	8	8	0	0
4	G	6	8	8	0	0
4	H	12	16	16	0	0
5	A	74	0	0	0	0
5	B	21	0	0	0	0
5	C	17	0	0	0	0
5	D	27	0	0	0	0
5	E	53	0	0	0	0
5	F	74	0	0	0	0
5	G	41	0	0	0	0
5	H	18	0	0	0	0
All	All	11470	32	11327	298	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 13.

All (298) 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:H:102:ILE:HG22	1:H:127:LEU:HD11	1.34	1.07
1:E:166:VAL:HG22	1:E:175:LEU:HB2	1.42	0.99
1:B:170:VAL:HG13	1:B:171:VAL:H	1.30	0.96
1:H:102:ILE:CG2	1:H:127:LEU:HD11	1.96	0.95
1:G:224:SER:HA	1:G:226:LEU:H	1.29	0.95
1:G:166:VAL:CG2	1:G:175:LEU:HB2	1.99	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:ASN:O	1:C:232:ILE:HD12	1.69	0.93
1:G:166:VAL:HG22	1:G:175:LEU:HB2	1.48	0.92
1:E:166:VAL:CG2	1:E:175:LEU:HB2	1.99	0.92
1:D:223:GLN:OE1	1:E:222:VAL:HA	1.71	0.91
1:A:124:VAL:HG23	1:A:125:PRO:HD3	1.54	0.87
1:C:229:LEU:O	1:C:233:LEU:HD23	1.76	0.84
1:C:80:LEU:O	1:C:84:LEU:HD23	1.78	0.84
1:C:100:ASP:O	1:C:102:ILE:HG22	1.77	0.84
1:H:257:ASP:OD1	1:H:259:THR:HG22	1.78	0.84
1:F:153:ARG:HG2	1:F:188:LEU:HD23	1.59	0.82
1:F:118:GLY:O	1:F:122:SER:HB2	1.80	0.81
1:G:223:GLN:O	1:G:225:PHE:HB3	1.80	0.80
1:C:141:LEU:HB2	1:C:159:PRO:HG2	1.63	0.80
1:G:130:ILE:HA	1:G:168:MET:HG2	1.62	0.79
1:H:141:LEU:HB2	1:H:159:PRO:HB2	1.64	0.79
1:B:72:LEU:HB3	1:B:264:ILE:HD11	1.66	0.78
1:C:135:ILE:HG12	1:C:164:LEU:HD23	1.66	0.78
1:H:103:LYS:HD2	1:H:127:LEU:HD12	1.66	0.78
1:A:139:GLN:NE2	1:E:139:GLN:OE1	2.18	0.77
1:E:274:PHE:CE1	1:E:275:VAL:HG23	2.19	0.77
1:E:267:LEU:HD13	1:E:274:PHE:CD2	2.20	0.77
1:D:215:LEU:HD21	1:D:219:VAL:HB	1.67	0.77
1:C:88:GLY:O	1:C:92:ILE:HG12	1.86	0.75
1:B:170:VAL:HG13	1:B:171:VAL:N	2.02	0.75
1:D:102:ILE:HG22	1:D:127:LEU:HD11	1.69	0.74
1:D:70:ASP:O	1:D:71:LEU:HB2	1.87	0.74
1:C:84:LEU:HD22	1:C:252:ILE:CD1	2.17	0.73
1:A:235:LYS:NZ	1:B:202:GLY:O	2.20	0.73
1:A:170:VAL:HG23	1:C:127:LEU:HA	1.71	0.72
1:A:124:VAL:CG2	1:A:125:PRO:HD3	2.21	0.70
1:A:192:ASP:OD1	1:A:196:ARG:N	2.24	0.70
1:F:192:ASP:OD1	1:F:196:ARG:N	2.23	0.69
1:A:99:LEU:HD13	1:A:132:ASP:HA	1.73	0.69
1:D:84:LEU:HD23	1:D:252:ILE:CD1	2.22	0.69
1:G:224:SER:HA	1:G:226:LEU:N	2.05	0.69
1:A:153:ARG:HG2	1:A:188:LEU:HD23	1.75	0.69
1:B:170:VAL:CG1	1:B:171:VAL:H	2.06	0.68
1:B:71[A]:LEU:HD13	3:B:307:CL:CL	2.31	0.68
1:D:124:VAL:N	1:D:125:PRO:HD2	2.09	0.68
1:F:141:LEU:HB2	1:F:159:PRO:HG2	1.76	0.68
1:E:125:PRO:O	1:E:127:LEU:N	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:ASN:OD1	1:B:170:VAL:HG11	1.94	0.67
1:G:128:ASN:O	1:G:129:ASN:HB2	1.93	0.67
1:H:257:ASP:CG	1:H:259:THR:HG22	2.15	0.67
1:B:99:LEU:HD11	1:B:103:LYS:HE3	1.76	0.67
1:C:155:TYR:CE1	1:C:186:GLU:HG3	2.30	0.66
1:E:181:LEU:HD23	1:E:241:ILE:HG21	1.75	0.66
1:F:121:THR:HB	1:F:127:LEU:CD1	2.24	0.66
1:C:221:PRO:HG2	1:C:226:LEU:HB2	1.78	0.66
1:B:72:LEU:HB3	1:B:264:ILE:CD1	2.26	0.65
1:E:141:LEU:HB2	1:E:159:PRO:HG2	1.77	0.65
1:E:186:GLU:HG2	1:E:203:ASP:N	2.11	0.65
1:H:102:ILE:HG22	1:H:127:LEU:CD1	2.20	0.64
1:G:171:VAL:O	1:G:171:VAL:HG12	1.98	0.63
1:B:263:ASN:OD1	1:F:64:LEU:HA	1.98	0.63
1:B:141:LEU:HB2	1:B:159:PRO:HG2	1.81	0.63
1:G:231:GLY:O	1:G:235:LYS:HG2	1.99	0.62
1:A:141:LEU:HB2	1:A:159:PRO:HG2	1.82	0.62
1:A:172:GLY:O	1:G:193:ASN:HA	1.99	0.62
1:F:64:LEU:N	1:F:65:PRO:CD	2.63	0.62
1:H:155:TYR:CE1	1:H:186:GLU:HG3	2.35	0.62
1:D:123:SER:C	1:D:125:PRO:HD2	2.20	0.61
1:C:135:ILE:HG12	1:C:164:LEU:CD2	2.30	0.61
1:B:71[A]:LEU:HA	3:B:307:CL:CL	2.37	0.61
1:C:101:VAL:HG11	1:C:236:VAL:CG1	2.30	0.61
1:H:153:ARG:HG2	1:H:188:LEU:HD23	1.81	0.61
1:D:153:ARG:HG2	1:D:188:LEU:HD23	1.83	0.60
1:D:141:LEU:HB2	1:D:159:PRO:HB2	1.82	0.60
1:C:257:ASP:OD1	1:C:259:THR:HG22	2.00	0.60
1:F:153:ARG:HG2	1:F:188:LEU:CD2	2.29	0.60
1:B:124:VAL:N	1:B:125:PRO:HD2	2.17	0.60
1:E:274:PHE:CD1	1:E:275:VAL:HG23	2.37	0.60
1:H:215:LEU:HD23	1:H:221:PRO:HD3	1.83	0.60
1:C:180:LYS:HB2	1:C:212:LYS:HB2	1.84	0.59
1:F:121:THR:HB	1:F:127:LEU:HD13	1.83	0.59
1:C:70:ASP:C	1:C:72:LEU:H	2.06	0.59
1:D:123:SER:CB	1:D:125:PRO:HD2	2.33	0.59
1:F:154:LEU:HG	1:F:268:LEU:HD21	1.85	0.58
1:F:186:GLU:HG2	1:F:203:ASP:N	2.18	0.58
1:D:97:PRO:O	1:D:101:VAL:HG23	2.03	0.58
1:A:153:ARG:HG2	1:A:188:LEU:CD2	2.33	0.58
1:C:94:GLU:OE2	1:C:138:PRO:HD3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:175:LEU:HD21	1:G:220:THR:O	2.03	0.58
1:G:101:VAL:HG21	1:G:240:LEU:HD21	1.85	0.57
1:H:90:LEU:HD22	1:H:138:PRO:HB2	1.85	0.57
1:G:141:LEU:HB2	1:G:159:PRO:HG2	1.86	0.57
1:A:186:GLU:HG2	1:A:203:ASP:N	2.20	0.57
1:D:124:VAL:N	1:D:125:PRO:CD	2.68	0.57
1:C:186:GLU:O	1:C:201:LEU:HD12	2.05	0.57
1:G:165:ASN:ND2	1:G:176:GLN:HG2	2.20	0.56
1:D:84:LEU:HD23	1:D:252:ILE:HD12	1.87	0.56
1:G:153:ARG:HG2	1:G:188:LEU:HD23	1.87	0.56
1:G:153:ARG:HD2	1:G:186:GLU:OE2	2.05	0.56
1:E:186:GLU:HG2	1:E:203:ASP:H	1.68	0.56
1:G:128:ASN:O	1:G:129:ASN:CB	2.54	0.56
1:D:132:ASP:OD1	1:D:167:ASN:HB3	2.04	0.56
1:F:197:ILE:HD11	1:F:269:ILE:HD12	1.87	0.56
1:A:99:LEU:CD1	1:A:132:ASP:HA	2.36	0.55
1:A:126:LEU:HD12	1:A:168:MET:HE3	1.88	0.55
1:C:132:ASP:OD1	1:C:167:ASN:HB3	2.06	0.55
1:C:101:VAL:HG11	1:C:236:VAL:HG11	1.89	0.55
1:E:146:VAL:CG2	1:E:155:TYR:HB2	2.36	0.55
1:G:177:LEU:HD23	1:G:215:LEU:HA	1.87	0.55
1:H:101:VAL:HG21	1:H:240:LEU:HD21	1.89	0.55
1:H:127:LEU:CD2	1:H:232:ILE:HD13	2.36	0.55
1:G:245:VAL:O	1:G:249:VAL:HG23	2.07	0.54
1:H:99:LEU:O	1:H:103:LYS:HG2	2.07	0.54
1:B:218:GLY:O	1:B:219:VAL:CB	2.56	0.54
1:E:132:ASP:OD1	1:E:167:ASN:HB3	2.08	0.54
1:A:211:LEU:C	1:A:212:LYS:HD2	2.27	0.54
1:C:241:ILE:O	1:C:245:VAL:HG23	2.08	0.54
1:G:166:VAL:HG23	1:G:166:VAL:O	2.07	0.53
1:D:274:PHE:C	1:D:274:PHE:CD1	2.80	0.53
1:C:171:VAL:HG12	1:C:171:VAL:O	2.07	0.53
1:D:226:LEU:O	1:D:230:THR:HG23	2.08	0.53
1:E:223:GLN:O	1:E:226:LEU:N	2.41	0.53
1:F:124:VAL:CG1	1:F:127:LEU:HD12	2.38	0.53
1:C:215:LEU:CD2	1:C:221:PRO:HD3	2.39	0.53
1:D:274:PHE:CE1	1:D:275:VAL:HG23	2.44	0.53
1:C:178:ALA:HB2	1:C:216:LEU:HD21	1.91	0.53
1:G:221:PRO:O	1:G:222:VAL:CB	2.56	0.53
1:C:257:ASP:CG	1:C:259:THR:HG22	2.29	0.52
1:D:221:PRO:O	1:D:222:VAL:O	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:166:VAL:O	1:E:166:VAL:HG23	2.09	0.52
1:A:126:LEU:HD12	1:A:168:MET:CE	2.39	0.52
1:C:76:PHE:CE2	1:C:80:LEU:HD11	2.46	0.51
1:A:211:LEU:O	1:A:212:LYS:HD2	2.10	0.51
1:C:84:LEU:HD22	1:C:252:ILE:HD12	1.92	0.51
1:D:70:ASP:O	1:D:71:LEU:CB	2.56	0.51
1:E:274:PHE:HD1	1:E:275:VAL:N	2.09	0.51
1:C:130:ILE:O	1:C:132:ASP:N	2.41	0.51
1:D:165:ASN:ND2	1:D:176:GLN:HG2	2.25	0.51
1:F:130:ILE:HG12	1:F:168:MET:HE2	1.93	0.51
1:G:174:LEU:O	1:G:218:GLY:HA3	2.11	0.51
1:C:94:GLU:OE2	1:C:138:PRO:CD	2.58	0.51
1:E:267:LEU:CD1	1:E:274:PHE:CD2	2.93	0.50
1:G:224:SER:CA	1:G:226:LEU:H	2.10	0.50
1:H:97:PRO:O	1:H:101:VAL:HG23	2.11	0.50
1:D:166:VAL:HB	1:D:175:LEU:HB3	1.92	0.50
1:C:130:ILE:O	1:C:167:ASN:O	2.29	0.50
1:E:267:LEU:HB3	1:E:274:PHE:HD2	1.76	0.50
1:G:166:VAL:HG21	1:G:175:LEU:HB2	1.88	0.50
1:H:153:ARG:HG2	1:H:188:LEU:CD2	2.41	0.50
1:F:124:VAL:HG11	1:F:127:LEU:HD12	1.93	0.50
1:C:102:ILE:O	1:C:102:ILE:HG23	2.12	0.50
1:F:146:VAL:CG2	1:F:155:TYR:HB2	2.42	0.50
1:E:127:LEU:O	1:E:129:ASN:N	2.42	0.50
1:D:274:PHE:CE1	1:D:275:VAL:CG2	2.95	0.50
1:H:165:ASN:OD1	1:H:176:GLN:HG2	2.12	0.50
1:B:248:LEU:O	1:B:252:ILE:HG12	2.11	0.49
1:E:84:LEU:HD23	1:E:252:ILE:CD1	2.42	0.49
1:F:99:LEU:CD2	1:F:132:ASP:HA	2.42	0.49
1:B:72:LEU:HD12	1:B:267:LEU:CD1	2.41	0.49
1:G:153:ARG:HG2	1:G:188:LEU:CD2	2.42	0.49
1:C:101:VAL:HG11	1:C:236:VAL:HG13	1.94	0.49
1:D:88:GLY:O	1:D:92:ILE:HG12	2.12	0.49
1:D:155:TYR:CE1	1:D:186:GLU:HG3	2.48	0.49
1:E:66:SER:HA	1:E:67:ASN:C	2.33	0.49
1:G:193:ASN:OD1	1:G:194:GLN:HG2	2.13	0.49
1:A:102:ILE:CG2	1:A:127:LEU:HD11	2.42	0.48
1:D:224:SER:OG	1:E:221:PRO:HA	2.14	0.48
1:A:67:ASN:OD1	1:A:68:PRO:HD2	2.13	0.48
1:H:257:ASP:OD2	1:H:259:THR:HG22	2.14	0.48
1:B:83:GLY:HA3	1:B:252:ILE:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:181:LEU:HD22	1:E:241:ILE:HD12	1.95	0.48
1:B:71[B]:LEU:HG	1:B:75:LYS:NZ	2.29	0.48
1:D:153:ARG:HG2	1:D:188:LEU:CD2	2.44	0.48
1:F:155:TYR:CE1	1:F:186:GLU:HB3	2.48	0.48
1:B:219:VAL:O	1:B:220:THR:CB	2.62	0.47
1:C:84:LEU:HD22	1:C:252:ILE:HD13	1.92	0.47
1:F:186:GLU:HG2	1:F:203:ASP:H	1.77	0.47
1:C:100:ASP:O	1:C:102:ILE:N	2.48	0.47
1:E:65:PRO:HG2	1:E:71:LEU:HD21	1.96	0.47
1:G:69:THR:HG22	1:G:274:PHE:HB2	1.97	0.47
1:B:72:LEU:HD12	1:B:267:LEU:HD12	1.96	0.47
1:C:176:GLN:HB3	1:C:216:LEU:HD12	1.94	0.47
1:E:267:LEU:HB3	1:E:274:PHE:CD2	2.49	0.47
1:C:90:LEU:HD22	1:C:138:PRO:HB2	1.96	0.47
1:F:121:THR:HB	1:F:127:LEU:HD12	1.95	0.47
1:D:223:GLN:HB2	1:E:221:PRO:O	2.15	0.47
1:G:179:VAL:HA	1:G:212:LYS:O	2.14	0.47
1:H:177:LEU:HD23	1:H:213:ILE:CG2	2.45	0.47
1:D:159:PRO:HA	1:D:182:ASN:OD1	2.16	0.46
1:B:124:VAL:N	1:B:125:PRO:CD	2.78	0.46
1:F:146:VAL:HG22	1:F:155:TYR:HB2	1.98	0.46
1:G:180:LYS:HB2	1:G:212:LYS:HB2	1.98	0.46
1:H:100:ASP:O	1:H:104:SER:HB2	2.16	0.46
1:H:101:VAL:O	1:H:104:SER:HB3	2.15	0.46
1:A:126:LEU:CD1	1:A:168:MET:HE1	2.44	0.46
1:B:153:ARG:HD2	1:B:186:GLU:OE2	2.16	0.46
1:E:126:LEU:O	1:E:127:LEU:CB	2.63	0.46
1:E:67:ASN:HA	1:E:68:PRO:HD3	1.86	0.46
1:A:129:ASN:OD1	1:C:170:VAL:HG21	2.16	0.45
1:B:88:GLY:O	1:B:92:ILE:HG13	2.15	0.45
1:C:164:LEU:HB2	1:C:177:LEU:HB2	1.98	0.45
1:G:166:VAL:HG22	1:G:175:LEU:CB	2.34	0.45
1:G:141:LEU:HD12	1:G:141:LEU:N	2.31	0.45
1:C:141:LEU:CB	1:C:159:PRO:HG2	2.40	0.45
1:B:72:LEU:HD13	1:B:264:ILE:HD13	1.97	0.45
1:D:215:LEU:CD2	1:D:219:VAL:HB	2.43	0.45
1:G:224:SER:HB3	1:G:227:ASP:H	1.82	0.45
1:E:274:PHE:HD1	1:E:274:PHE:C	2.20	0.45
1:F:219:VAL:O	1:F:219:VAL:HG12	2.16	0.45
1:G:69:THR:CG2	1:G:274:PHE:HB2	2.47	0.45
1:A:231:GLY:O	1:A:235:LYS:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:ILE:HA	1:B:165:ASN:O	2.17	0.45
1:B:192:ASP:OD1	1:B:196:ARG:N	2.50	0.45
1:E:165:ASN:OD1	1:E:176:GLN:HG2	2.18	0.44
1:H:124:VAL:HB	1:H:125:PRO:HD2	1.98	0.44
1:A:274:PHE:HD2	1:A:274:PHE:N	2.16	0.44
1:C:237:LEU:N	1:C:238:PRO:HD2	2.32	0.44
1:A:146:VAL:HG22	1:A:155:TYR:HB2	2.00	0.44
1:C:246:CYS:N	1:C:247:PRO:HD2	2.32	0.44
1:E:177:LEU:HD23	1:E:215:LEU:HA	1.99	0.44
1:D:141:LEU:HD12	1:D:141:LEU:N	2.33	0.44
1:E:229:LEU:O	1:E:233:LEU:HG	2.18	0.44
1:F:65:PRO:O	1:F:66:SER:C	2.56	0.44
1:G:166:VAL:CG2	1:G:166:VAL:O	2.66	0.44
1:H:179:VAL:HA	1:H:212:LYS:O	2.17	0.44
1:B:71[B]:LEU:HD12	1:B:71[B]:LEU:O	2.17	0.44
1:C:101:VAL:CG1	1:C:236:VAL:HG11	2.48	0.44
1:D:219:VAL:HG12	1:D:220:THR:N	2.33	0.44
1:E:222:VAL:O	1:E:225:PHE:HB3	2.18	0.44
1:B:96:ILE:CG2	1:B:240:LEU:HD13	2.47	0.44
1:E:274:PHE:CD1	1:E:274:PHE:C	2.91	0.44
1:G:237:LEU:HB3	1:G:238:PRO:HD3	1.99	0.43
1:A:186:GLU:HG2	1:A:203:ASP:H	1.83	0.43
1:F:181:LEU:HD23	1:F:241:ILE:HG21	1.99	0.43
1:A:124:VAL:HG23	1:A:125:PRO:CD	2.38	0.43
1:B:266:GLU:HB3	1:F:68:PRO:CG	2.48	0.43
1:D:229:LEU:O	1:D:233:LEU:HG	2.18	0.43
1:D:274:PHE:C	1:D:274:PHE:HD1	2.21	0.43
1:D:68:PRO:O	1:D:70:ASP:O	2.35	0.43
1:F:64:LEU:N	1:F:65:PRO:HD3	2.34	0.43
1:A:177:LEU:N	1:A:177:LEU:HD12	2.34	0.43
1:A:274:PHE:HD2	1:A:274:PHE:H	1.66	0.43
1:B:186:GLU:O	1:B:201:LEU:HD12	2.18	0.43
1:C:233:LEU:HD22	1:C:233:LEU:N	2.33	0.43
1:A:147:GLN:OE1	1:A:274:PHE:HD2	2.02	0.43
1:C:171:VAL:CG1	1:C:171:VAL:O	2.66	0.43
1:A:99:LEU:HD23	1:A:99:LEU:C	2.38	0.43
1:B:155:TYR:CE1	1:B:186:GLU:HG3	2.54	0.43
1:E:179:VAL:HA	1:E:212:LYS:O	2.18	0.43
1:G:125:PRO:HG2	1:G:126:LEU:H	1.83	0.43
1:B:246:CYS:HB2	1:B:247:PRO:HD3	2.00	0.43
1:B:83:GLY:CA	1:B:252:ILE:HD12	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:155:TYR:CE1	1:G:186:GLU:HG3	2.54	0.43
1:B:129:ASN:O	1:B:168:MET:HA	2.20	0.42
1:E:239:GLU:N	1:E:239:GLU:OE1	2.47	0.42
1:E:184:THR:HG21	1:H:208:PRO:HB2	2.00	0.42
1:C:94:GLU:HG2	1:C:135:ILE:O	2.19	0.42
1:A:192:ASP:OD1	1:A:195:GLY:N	2.52	0.42
1:D:132:ASP:OD1	1:D:167:ASN:CB	2.67	0.42
1:F:124:VAL:HG13	1:F:124:VAL:O	2.19	0.42
1:F:166:VAL:HB	1:F:175:LEU:HB3	2.01	0.42
1:F:177:LEU:HD12	1:F:177:LEU:N	2.34	0.42
1:B:157:THR:O	1:B:159:PRO:HD3	2.19	0.42
1:C:133:ILE:HA	1:C:165:ASN:O	2.20	0.42
1:C:188:LEU:N	1:C:188:LEU:HD12	2.34	0.42
1:D:131:LEU:HD23	1:D:167:ASN:ND2	2.34	0.42
1:H:259:THR:HG23	1:H:260:LEU:N	2.35	0.42
1:A:274:PHE:CD2	1:A:274:PHE:N	2.87	0.42
1:F:274:PHE:CD2	1:F:274:PHE:N	2.87	0.42
1:G:192:ASP:OD1	1:G:196:ARG:N	2.47	0.42
1:H:241:ILE:O	1:H:245:VAL:HG23	2.20	0.42
1:H:148:SER:OG	1:H:150:ASP:OD1	2.27	0.42
1:A:146:VAL:CG2	1:A:155:TYR:HB2	2.50	0.41
1:G:201:LEU:HD11	1:G:204:CYS:HB2	2.02	0.41
1:A:222:VAL:CG1	1:A:225:PHE:HB3	2.50	0.41
1:C:257:ASP:OD2	1:C:259:THR:HG22	2.20	0.41
1:B:137:ASP:N	1:B:138:PRO:CD	2.83	0.41
1:E:192:ASP:OD1	1:E:196:ARG:N	2.49	0.41
1:H:133:ILE:HA	1:H:165:ASN:O	2.21	0.41
1:A:124:VAL:N	1:A:125:PRO:CD	2.84	0.41
1:D:237:LEU:N	1:D:238:PRO:CD	2.84	0.41
1:C:99:LEU:O	1:C:99:LEU:HD23	2.21	0.41
1:D:133:ILE:HA	1:D:165:ASN:O	2.20	0.41
1:H:257:ASP:OD2	1:H:259:THR:CG2	2.69	0.41
1:H:124:VAL:HB	1:H:125:PRO:CD	2.51	0.41
1:E:274:PHE:CD1	1:E:275:VAL:N	2.88	0.41
1:A:225:PHE:CD2	1:C:222:VAL:HG23	2.56	0.41
1:C:179:VAL:HA	1:C:212:LYS:O	2.21	0.41
1:E:67:ASN:OD1	1:E:68:PRO:HD2	2.21	0.41
1:G:211:LEU:CD2	1:G:234:THR:HA	2.51	0.41
1:B:80:LEU:O	1:B:84:LEU:HG	2.21	0.40
1:H:80:LEU:HA	1:H:80:LEU:HD23	1.91	0.40
1:A:94:GLU:HG3	1:A:138:PRO:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:136:THR:HG23	1:E:165:ASN:ND2	2.36	0.40
1:B:71[B]:LEU:CD1	1:B:75:LYS:HZ2	2.35	0.40
1:C:141:LEU:HB2	1:C:159:PRO:CG	2.43	0.40
1:F:201:LEU:HD11	1:F:204:CYS:HB2	2.04	0.40
1:G:225:PHE:N	1:G:228:ASN:OD1	2.53	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	192/244 (79%)	183 (95%)	7 (4%)	2 (1%)	15	28
1	B	189/244 (78%)	174 (92%)	6 (3%)	9 (5%)	2	2
1	C	183/244 (75%)	171 (93%)	8 (4%)	4 (2%)	6	10
1	D	184/244 (75%)	173 (94%)	7 (4%)	4 (2%)	6	10
1	E	192/244 (79%)	183 (95%)	7 (4%)	2 (1%)	15	28
1	F	207/244 (85%)	196 (95%)	9 (4%)	2 (1%)	15	28
1	G	189/244 (78%)	174 (92%)	10 (5%)	5 (3%)	5	8
1	H	187/244 (77%)	182 (97%)	5 (3%)	0	100	100
All	All	1523/1952 (78%)	1436 (94%)	59 (4%)	28 (2%)	8	14

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	219	VAL
1	B	220	THR
1	D	222	VAL
1	F	66	SER
1	G	222	VAL

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Mol	Chain	Res	Type
1	B	170	VAL
1	C	101	VAL
1	E	127	LEU
1	A	103	LYS
1	A	125	PRO
1	B	217	ASN
1	B	221	PRO
1	C	71	LEU
1	C	126	LEU
1	C	128	ASN
1	G	104	SER
1	G	129	ASN
1	G	223	GLN
1	E	224	SER
1	F	106	GLY
1	B	70	ASP
1	B	126	LEU
1	B	171	VAL
1	D	220	THR
1	B	172	GLY
1	G	221	PRO
1	D	124	VAL
1	D	218	GLY

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	154/205 (75%)	152 (99%)	2 (1%)	69	87
1	B	143/205 (70%)	142 (99%)	1 (1%)	84	94
1	C	145/205 (71%)	144 (99%)	1 (1%)	84	94
1	D	140/205 (68%)	139 (99%)	1 (1%)	84	94
1	E	151/205 (74%)	150 (99%)	1 (1%)	84	94
1	F	166/205 (81%)	165 (99%)	1 (1%)	86	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	149/205 (73%)	148 (99%)	1 (1%)	84	94
1	H	147/205 (72%)	147 (100%)	0	100	100
All	All	1195/1640 (73%)	1187 (99%)	8 (1%)	84	94

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	250	ASN
1	A	274	PHE
1	B	259	THR
1	C	99	LEU
1	D	274	PHE
1	E	274	PHE
1	F	274	PHE
1	G	274	PHE

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

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 68 ligands modelled in this entry, 64 are monoatomic - leaving 4 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	$\# Z > 2$
4	GOL	H	302	-	5,5,5	1.09	0	5,5,5	1.01	0
4	GOL	C	301	-	5,5,5	1.23	0	5,5,5	0.70	0
4	GOL	G	301	-	5,5,5	1.24	0	5,5,5	0.62	0
4	GOL	H	301	-	5,5,5	1.34	1 (20%)	5,5,5	0.82	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	H	302	-	-	1/4/4/4	-
4	GOL	C	301	-	-	2/4/4/4	-
4	GOL	G	301	-	-	2/4/4/4	-
4	GOL	H	301	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	301	GOL	C3-C2	2.14	1.60	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	301	GOL	O1-C1-C2-C3
4	G	301	GOL	O1-C1-C2-O2
4	C	301	GOL	C1-C2-C3-O3
4	H	302	GOL	O1-C1-C2-O2
4	C	301	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	196/244 (80%)	-0.08	5 (2%) 56 59	14, 32, 66, 78	0
1	B	192/244 (78%)	0.04	7 (3%) 42 46	21, 36, 70, 106	0
1	C	187/244 (76%)	0.30	12 (6%) 19 20	25, 48, 71, 85	0
1	D	190/244 (77%)	0.09	9 (4%) 31 33	20, 38, 75, 99	0
1	E	196/244 (80%)	0.07	10 (5%) 28 29	16, 31, 72, 81	0
1	F	211/244 (86%)	-0.06	6 (2%) 53 56	14, 29, 64, 85	0
1	G	195/244 (79%)	0.13	12 (6%) 20 21	15, 36, 76, 84	0
1	H	191/244 (78%)	0.15	7 (3%) 41 45	23, 44, 61, 77	0
All	All	1558/1952 (79%)	0.08	68 (4%) 34 37	14, 37, 72, 106	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	221	PRO	6.2
1	G	220	THR	6.0
1	E	218	GLY	5.7
1	C	99	LEU	5.1
1	D	169	PRO	4.6
1	C	89	LEU	4.5
1	C	85	LEU	4.4
1	E	220	THR	4.4
1	C	93	LEU	4.4
1	E	219	VAL	4.2
1	G	169	PRO	4.0
1	G	173	SER	4.0
1	G	170	VAL	3.9
1	C	84	LEU	3.8
1	E	170	VAL	3.7
1	D	224	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	219	VAL	3.7
1	G	221	PRO	3.6
1	E	169	PRO	3.5
1	C	166	VAL	3.5
1	G	218	GLY	3.4
1	C	130	ILE	3.4
1	B	221	PRO	3.4
1	F	220	THR	3.3
1	H	84	LEU	3.2
1	A	218	GLY	3.1
1	H	222	VAL	3.1
1	C	128	ASN	3.0
1	G	172	GLY	3.0
1	G	107	GLY	2.9
1	A	221	PRO	2.9
1	B	224	SER	2.8
1	G	222	VAL	2.8
1	H	125	PRO	2.8
1	A	217	ASN	2.8
1	D	139	GLN	2.8
1	B	222	VAL	2.8
1	F	122	SER	2.7
1	D	173	SER	2.6
1	G	125	PRO	2.6
1	C	137	ASP	2.5
1	E	225	PHE	2.5
1	A	122	SER	2.5
1	E	125	PRO	2.5
1	C	90	LEU	2.4
1	F	64	LEU	2.4
1	E	217	ASN	2.4
1	B	124	VAL	2.4
1	A	220	THR	2.4
1	D	220	THR	2.4
1	C	174	LEU	2.3
1	D	225	PHE	2.3
1	E	65	PRO	2.3
1	B	278	VAL	2.3
1	C	222	VAL	2.3
1	D	125	PRO	2.2
1	F	123	SER	2.2
1	F	111	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	71[A]	LEU	2.2
1	G	225	PHE	2.2
1	G	217	ASN	2.1
1	D	221	PRO	2.1
1	H	102	ILE	2.1
1	D	222	VAL	2.1
1	F	195	GLY	2.1
1	H	141	LEU	2.0
1	H	129	ASN	2.0
1	H	89	LEU	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 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. 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	B-factors(Å ²)	Q<0.9
4	GOL	C	301	6/6	0.66	0.29	47,58,72,72	0
2	NA	A	306	1/1	0.68	0.17	66,66,66,66	0
2	NA	A	303	1/1	0.70	0.17	45,45,45,45	0
3	CL	B	307	1/1	0.70	0.30	63,63,63,63	0
2	NA	G	313	1/1	0.70	0.54	54,54,54,54	0
2	NA	E	307	1/1	0.72	0.16	62,62,62,62	0
4	GOL	H	301	6/6	0.74	0.21	45,58,68,70	0
2	NA	D	304	1/1	0.77	0.93	52,52,52,52	0
2	NA	D	301	1/1	0.77	0.24	78,78,78,78	0
2	NA	C	306	1/1	0.78	0.30	51,51,51,51	0
2	NA	H	307	1/1	0.79	0.18	75,75,75,75	0
2	NA	F	304	1/1	0.79	0.11	67,67,67,67	0
4	GOL	H	302	6/6	0.79	0.22	44,62,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NA	C	304	1/1	0.80	0.12	57,57,57,57	0
2	NA	G	310	1/1	0.80	0.19	55,55,55,55	0
2	NA	G	312	1/1	0.82	0.31	60,60,60,60	0
4	GOL	G	301	6/6	0.84	0.25	42,51,62,66	0
2	NA	A	304	1/1	0.85	0.19	45,45,45,45	0
2	NA	C	308	1/1	0.86	0.11	69,69,69,69	0
2	NA	G	307	1/1	0.86	0.17	51,51,51,51	0
2	NA	H	306	1/1	0.86	0.22	65,65,65,65	0
2	NA	E	308	1/1	0.87	0.18	53,53,53,53	0
2	NA	B	302	1/1	0.87	0.13	64,64,64,64	0
2	NA	B	301	1/1	0.87	0.21	48,48,48,48	0
2	NA	F	302	1/1	0.88	0.17	49,49,49,49	0
2	NA	C	305	1/1	0.88	0.38	58,58,58,58	0
2	NA	G	303	1/1	0.88	0.14	42,42,42,42	0
2	NA	H	304	1/1	0.90	0.23	56,56,56,56	0
2	NA	F	305	1/1	0.91	0.16	43,43,43,43	0
2	NA	A	305	1/1	0.91	0.14	47,47,47,47	0
2	NA	G	302	1/1	0.91	0.43	63,63,63,63	0
2	NA	H	308	1/1	0.91	0.34	65,65,65,65	0
2	NA	C	303	1/1	0.91	0.23	45,45,45,45	0
2	NA	B	305	1/1	0.92	0.36	43,43,43,43	0
2	NA	D	303	1/1	0.92	0.12	68,68,68,68	0
2	NA	F	301	1/1	0.92	0.15	41,41,41,41	0
2	NA	G	314	1/1	0.92	0.10	46,46,46,46	0
2	NA	E	303	1/1	0.93	0.11	54,54,54,54	0
2	NA	A	308	1/1	0.93	0.27	51,51,51,51	0
2	NA	H	309	1/1	0.93	0.68	52,52,52,52	0
2	NA	E	309	1/1	0.93	0.09	42,42,42,42	0
2	NA	E	301	1/1	0.93	0.33	39,39,39,39	0
2	NA	D	302	1/1	0.93	0.11	57,57,57,57	0
2	NA	G	309	1/1	0.94	0.19	48,48,48,48	0
2	NA	G	304	1/1	0.94	0.21	65,65,65,65	0
2	NA	B	306	1/1	0.94	0.15	46,46,46,46	0
2	NA	C	309	1/1	0.94	0.19	60,60,60,60	0
2	NA	E	302	1/1	0.94	0.16	49,49,49,49	0
2	NA	E	305	1/1	0.94	0.29	51,51,51,51	0
2	NA	C	307	1/1	0.95	0.12	53,53,53,53	0
2	NA	A	311	1/1	0.95	0.17	47,47,47,47	0
2	NA	H	305	1/1	0.95	0.11	41,41,41,41	0
2	NA	A	301	1/1	0.95	0.32	49,49,49,49	0
2	NA	A	307	1/1	0.95	0.10	42,42,42,42	0
2	NA	C	302	1/1	0.95	0.30	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NA	B	304	1/1	0.95	0.11	36,36,36,36	0
2	NA	G	311	1/1	0.95	0.18	57,57,57,57	0
2	NA	A	309	1/1	0.96	0.06	49,49,49,49	0
2	NA	G	306	1/1	0.96	0.27	55,55,55,55	0
2	NA	B	303	1/1	0.96	0.17	46,46,46,46	0
2	NA	H	303	1/1	0.96	0.18	36,36,36,36	0
2	NA	F	303	1/1	0.96	0.35	47,47,47,47	0
2	NA	G	305	1/1	0.96	0.23	43,43,43,43	0
2	NA	A	302	1/1	0.96	0.15	52,52,52,52	0
2	NA	A	310	1/1	0.96	0.20	44,44,44,44	0
2	NA	G	308	1/1	0.98	0.11	58,58,58,58	0
2	NA	E	304	1/1	0.98	0.08	48,48,48,48	0
2	NA	E	306	1/1	0.99	0.18	42,42,42,42	0

6.5 Other polymers ⓘ

There are no such residues in this entry.