



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2026 – 06:11 PM UTC

PDB ID : 6BAQ / pdb_00006baq
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

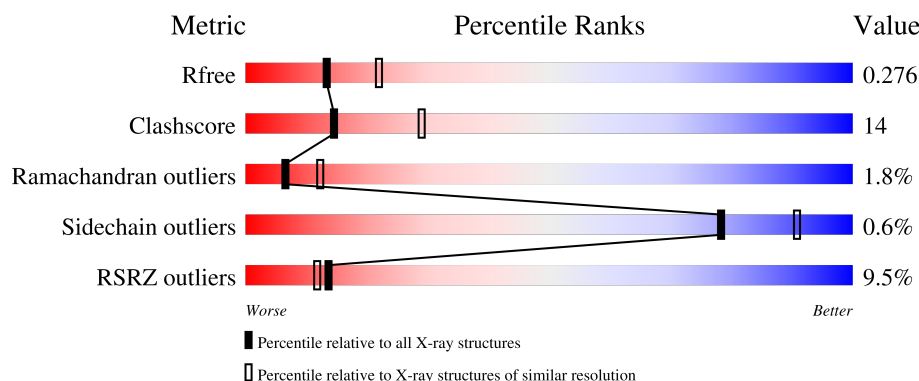
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 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 $\leq 5\%$. 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	6% 64% 15% • 20%
1	B	244	5% 57% 20% • 21%
1	C	244	12% 52% 23% • 23%
1	D	244	8% 59% 17% • 22%
1	E	244	8% 60% 20% • 20%

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Mol	Chain	Length	Quality of chain
1	F	244	
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
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 (CCD ID: NA) (formula: Na).

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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 4 is GLYCEROL (CCD ID: 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		

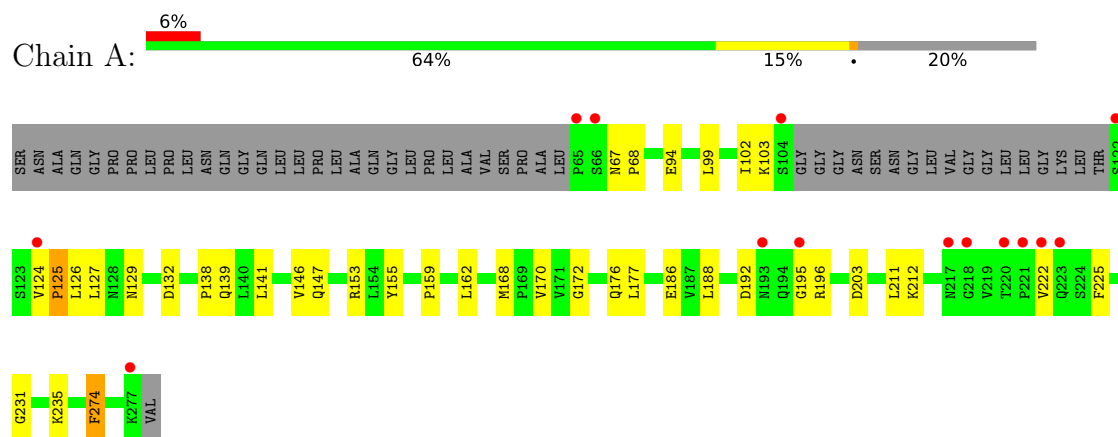
- Molecule 5 is water.

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		

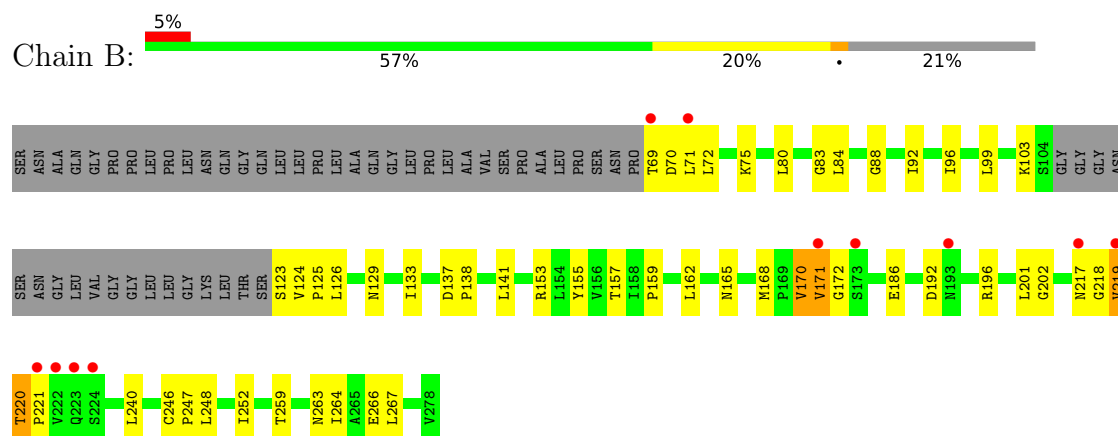
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

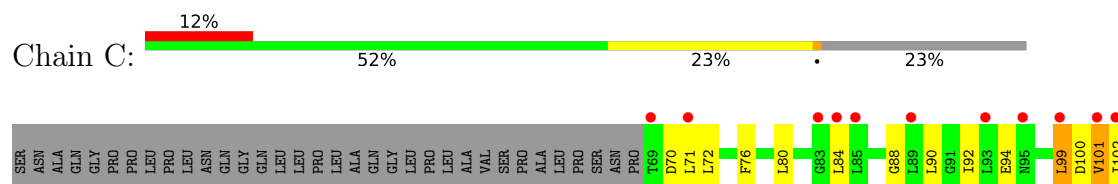
- Molecule 1: BPI fold-containing family A member 1

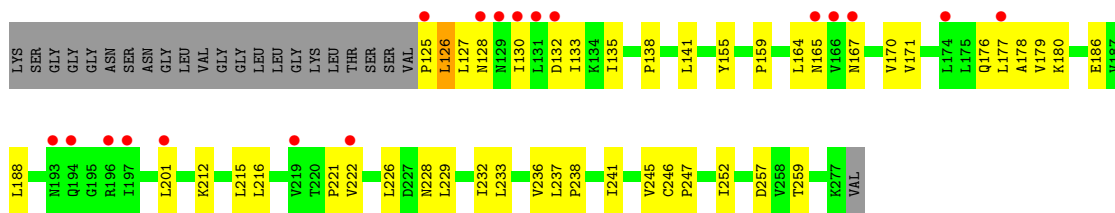


- Molecule 1: BPI fold-containing family A member 1

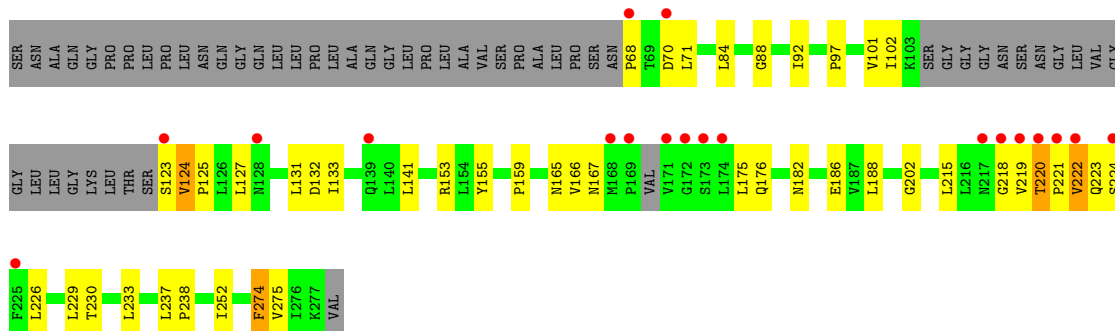


- Molecule 1: BPI fold-containing family A member 1

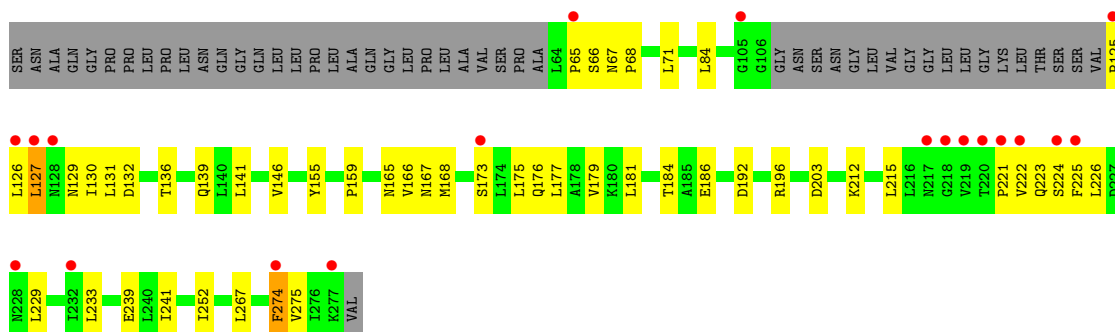




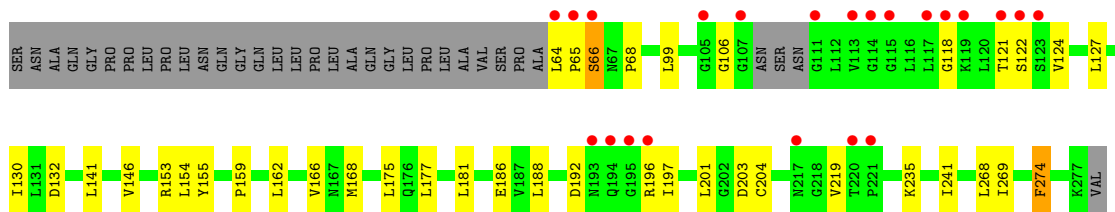
• Molecule 1: BPI fold-containing family A member 1



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

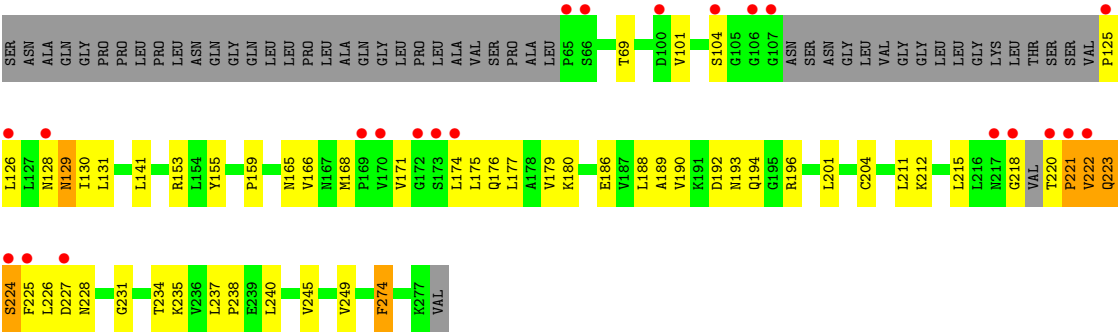


• Molecule 1: BPI fold-containing family A member 1

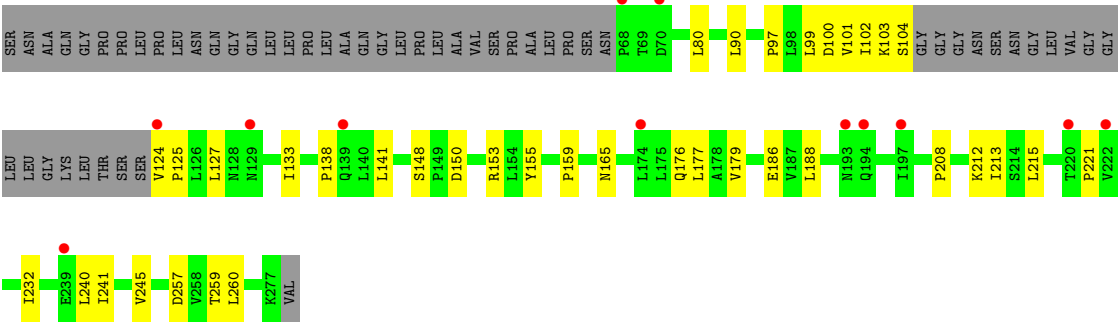


• Molecule 1: BPI fold-containing family A member 1





● 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 41.79 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.8 (41.79-2.50) 94.4 (41.79-2.50)	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 (3.08%)	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)	0.35 , 63.7	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: CL, NA, GOL

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	0.39	0/1419	0.70	0/1944
1	B	0.38	0/1377	0.67	0/1886
1	C	0.34	0/1346	0.60	0/1845
1	D	0.37	0/1352	0.64	0/1852
1	E	0.38	0/1412	0.70	0/1931
1	F	0.41	0/1520	0.68	0/2079
1	G	0.38	0/1398	0.67	2/1909 (0.1%)
1	H	0.32	0/1376	0.55	0/1887
All	All	0.37	0/11200	0.65	2/15333 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	224	SER	CA-C-N	6.00	132.51	121.70
1	G	224	SER	C-N-CA	6.00	132.51	121.70

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	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1360	0	1365	43	0
1	C	1329	0	1358	54	0
1	D	1335	0	1350	39	0
1	E	1394	0	1420	44	0
1	F	1501	0	1570	34	0
1	G	1380	0	1400	43	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	314	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 14.

All (314) 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:H:257:ASP:CG	1:H:259:THR:HG22	2.15	0.71
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:125:PRO:O	1:E:127:LEU:N	2.26	0.67
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: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:D:123:SER:C	1:D:125:PRO:HD2	2.20	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:C:70:ASP:C	1:C:72:LEU:H	2.06	0.64
1:G:171:VAL:HG12	1:G:171:VAL:O	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: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:141:LEU:HB2	1:D:159:PRO:HB2	1.82	0.60
1:D:153:ARG:HG2	1:D:188:LEU:HD23	1.83	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:A:211:LEU:C	1:A:212:LYS:HD2	2.27	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:D:274:PHE:CD1	1:D:274:PHE:C	2.80	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:257:ASP:CG	1:C:259:THR:HG22	2.29	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:C:101:VAL:HG11	1:C:236:VAL:HG11	1.89	0.55
1:C:132:ASP:OD1	1:C:167:ASN:HB3	2.06	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:A:126:LEU:CD1	1:A:168:MET:HE1	2.36	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:C:241:ILE:O	1:C:245:VAL:HG23	2.08	0.54
1:F:130:ILE:HG12	1:F:168:MET:HE2	1.89	0.54
1:E:66:SER:HA	1:E:67:ASN:C	2.33	0.53
1:G:166:VAL:HG23	1:G:166:VAL:O	2.07	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:221:PRO:O	1:G:222:VAL:CB	2.56	0.53
1:D:221:PRO:O	1:D:222:VAL:O	2.27	0.52
1:E:166:VAL:HG23	1:E:166:VAL:O	2.09	0.52
1:F:130:ILE:CG1	1:F:168:MET:HE2	2.40	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:H:148:SER:OG	1:H:150:ASP:OD1	2.27	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: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:HG23	1:C:102:ILE:O	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:E:274:PHE:HD1	1:E:274:PHE:C	2.20	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:E:274:PHE:CD1	1:E:274:PHE:C	2.91	0.49
1:D:155:TYR:CE1	1:D:186:GLU:HG3	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:65:PRO:O	1:F:66:SER:C	2.56	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:B:83:GLY:HA3	1:B:252:ILE:HD12	1.96	0.48
1:D:274:PHE:C	1:D:274:PHE:HD1	2.21	0.48
1:E:181:LEU:HD22	1:E:241:ILE:HD12	1.95	0.48
1:H:257:ASP:OD2	1:H:259:THR:HG22	2.14	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:A:99:LEU:HD23	1:A:99:LEU:C	2.38	0.47
1:B:219:VAL:O	1:B:220:THR:CB	2.62	0.47
1:C:70:ASP:C	1:C:72:LEU:N	2.72	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:D:223:GLN:HB2	1:E:221:PRO:O	2.15	0.47
1:F:121:THR:HB	1:F:127:LEU:HD12	1.95	0.47
1:G:179:VAL:HA	1:G:212:LYS:O	2.14	0.47
1:A:126:LEU:HD12	1:A:168:MET:HE3	1.97	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:B:153:ARG:HD2	1:B:186:GLU:OE2	2.16	0.46
1:E:67:ASN:HA	1:E:68:PRO:HD3	1.86	0.46
1:E:126:LEU:O	1:E:127:LEU:CB	2.63	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:E:168:MET:HE3	1:E:173:SER:HB2	1.98	0.45
1:G:166:VAL:HG22	1:G:175:LEU:CB	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:219:VAL:HG12	1:F:219:VAL:O	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
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: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:B:170:VAL:O	1:B:171:VAL:C	2.60	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:B:162:LEU:HD12	1:B:162:LEU:C	2.43	0.44
1:D:202:GLY:O	1:F:235:LYS:NZ	2.42	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:E:130:ILE:O	1:E:131:LEU:C	2.59	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:HD12	1:A:177:LEU:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:LEU:N	1:C:233:LEU:HD22	2.33	0.43
1:A:147:GLN:OE1	1:A:274:PHE:HD2	2.02	0.43
1:C:171:VAL:O	1:C:171:VAL:CG1	2.66	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:83:GLY:CA	1:B:252:ILE:HD12	2.49	0.43
1:B:246:CYS:HB2	1:B:247:PRO:HD3	2.00	0.43
1:G:155:TYR:CE1	1:G:186:GLU:HG3	2.54	0.43
1:A:162:LEU:C	1:A:162:LEU:HD12	2.44	0.42
1:F:162:LEU:C	1:F:162:LEU:HD12	2.44	0.42
1:B:129:ASN:O	1:B:168:MET:HA	2.20	0.42
1:E:184:THR:HG21	1:H:208:PRO:HB2	2.00	0.42
1:E:239:GLU:OE1	1:E:239:GLU:N	2.47	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:O	1:F:124:VAL:HG13	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:123:SER:C	1:B:125:PRO:HD2	2.44	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:HD12	1:C:188:LEU:N	2.34	0.42
1:D:131:LEU:HD23	1:D:167:ASN:ND2	2.34	0.42
1:A:274:PHE:N	1:A:274:PHE:CD2	2.87	0.42
1:B:69:THR:C	1:B:71[B]:LEU:H	2.28	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:G:130:ILE:O	1:G:131:LEU:C	2.63	0.42
1:H:259:THR:HG23	1:H:260:LEU:N	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:LEU:HD23	1:C:99:LEU:O	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:A:225:PHE:CD2	1:C:222:VAL:HG23	2.56	0.41
1:B:83:GLY:C	1:B:252:ILE:HD12	2.45	0.41
1:C:125:PRO:O	1:C:126:LEU:C	2.64	0.41
1:E:274:PHE:CD1	1:E:275:VAL:N	2.88	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:HD23	1:H:80:LEU:HA	1.91	0.40
1:A:94:GLU:HG3	1:A:138:PRO:HG3	2.03	0.40
1:A:176:GLN:C	1:A:177:LEU:HD12	2.47	0.40
1:E:136:THR:HG23	1:E:165:ASN:ND2	2.36	0.40
1:G:189:ALA:C	1:G:190:VAL:HG23	2.46	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%)	12	24
1	B	189/244 (78%)	174 (92%)	6 (3%)	9 (5%)	2	2
1	C	183/244 (75%)	171 (93%)	8 (4%)	4 (2%)	5	9
1	D	184/244 (75%)	173 (94%)	7 (4%)	4 (2%)	5	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	192/244 (79%)	183 (95%)	7 (4%)	2 (1%)	12	24
1	F	207/244 (85%)	196 (95%)	9 (4%)	2 (1%)	12	24
1	G	189/244 (78%)	174 (92%)	10 (5%)	5 (3%)	4	7
1	H	187/244 (77%)	182 (97%)	5 (3%)	0	100	100
All	All	1523/1952 (78%)	1436 (94%)	59 (4%)	28 (2%)	6	12

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
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%)	153 (99%)	1 (1%)	78	91
1	B	143/205 (70%)	142 (99%)	1 (1%)	76	89
1	C	145/205 (71%)	144 (99%)	1 (1%)	76	89
1	D	140/205 (68%)	139 (99%)	1 (1%)	76	89
1	E	151/205 (74%)	150 (99%)	1 (1%)	76	89
1	F	166/205 (81%)	165 (99%)	1 (1%)	78	91
1	G	149/205 (73%)	148 (99%)	1 (1%)	76	89
1	H	147/205 (72%)	147 (100%)	0	100	100
All	All	1195/1640 (73%)	1188 (99%)	7 (1%)	78	91

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	ASN
1	A	176	GLN
1	A	198	HIS
1	C	262	HIS
1	C	263	ASN
1	D	129	ASN
1	E	95	ASN

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Mol	Chain	Res	Type
1	E	165	ASN
1	F	95	ASN
1	F	152	HIS
1	H	262	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	301	-	5,5,5	1.43	2 (40%)	5,5,5	0.88	0
4	GOL	G	301	-	5,5,5	1.31	1 (20%)	5,5,5	0.68	0
4	GOL	H	302	-	5,5,5	1.16	0	5,5,5	1.08	0
4	GOL	C	301	-	5,5,5	1.31	0	5,5,5	0.75	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	301	-	-	0/4/4/4	-
4	GOL	G	301	-	-	2/4/4/4	-
4	GOL	H	302	-	-	1/4/4/4	-
4	GOL	C	301	-	-	2/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	301	GOL	C3-C2	2.29	1.60	1.51
4	H	301	GOL	C1-C2	2.12	1.59	1.51
4	G	301	GOL	C3-C2	2.03	1.59	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	H	302	GOL	O1-C1-C2-O2
4	C	301	GOL	O2-C2-C3-O3
4	C	301	GOL	C1-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%)	0.15	14 (7%) 22 19	14, 32, 66, 78	0
1	B	192/244 (78%)	0.43	11 (5%) 29 26	21, 36, 70, 106	1 (0%)
1	C	187/244 (76%)	0.94	29 (15%) 5 4	25, 48, 71, 85	0
1	D	190/244 (77%)	0.47	19 (10%) 12 10	20, 38, 75, 99	0
1	E	196/244 (80%)	0.25	19 (9%) 13 11	16, 31, 72, 81	0
1	F	211/244 (86%)	0.13	22 (10%) 11 10	14, 29, 64, 85	0
1	G	195/244 (79%)	0.42	22 (11%) 10 8	15, 36, 76, 84	0
1	H	191/244 (78%)	0.52	12 (6%) 26 23	23, 44, 61, 77	0
All	All	1558/1952 (79%)	0.40	148 (9%) 14 12	14, 37, 72, 106	1 (0%)

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	71[A]	LEU	14.8
1	G	220	THR	5.7
1	E	218	GLY	5.3
1	G	125	PRO	5.1
1	F	122	SER	5.0
1	D	173	SER	4.8
1	D	224	SER	4.8
1	B	222	VAL	4.5
1	E	219	VAL	4.4
1	F	220	THR	4.3
1	F	105	GLY	4.2
1	D	222	VAL	4.0
1	B	221	PRO	3.9
1	F	107	GLY	3.8
1	A	221	PRO	3.8
1	G	221	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
1	E	220	THR	3.7
1	G	222	VAL	3.7
1	C	99	LEU	3.7
1	D	221	PRO	3.7
1	F	119	LYS	3.7
1	A	218	GLY	3.7
1	G	225	PHE	3.7
1	B	219	VAL	3.6
1	E	126	LEU	3.6
1	E	221	PRO	3.6
1	C	174	LEU	3.6
1	D	217	ASN	3.6
1	E	128	ASN	3.6
1	E	125	PRO	3.6
1	H	124	VAL	3.5
1	F	123	SER	3.5
1	B	217	ASN	3.5
1	G	126	LEU	3.5
1	G	169	PRO	3.4
1	G	218	GLY	3.4
1	F	66	SER	3.4
1	D	68	PRO	3.4
1	E	228	ASN	3.4
1	A	220	THR	3.4
1	D	225	PHE	3.3
1	C	197	ILE	3.3
1	B	193	ASN	3.3
1	C	102	ILE	3.3
1	C	222	VAL	3.3
1	F	121	THR	3.3
1	D	123	SER	3.3
1	E	225	PHE	3.3
1	D	139	GLN	3.3
1	G	174	LEU	3.2
1	B	224	SER	3.2
1	C	128	ASN	3.2
1	F	193	ASN	3.2
1	H	193	ASN	3.2
1	E	224	SER	3.2
1	H	68	PRO	3.1
1	D	171	VAL	3.1
1	C	93	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	132	ASP	3.1
1	G	227	ASP	3.1
1	F	111	GLY	3.1
1	B	171	VAL	3.1
1	C	194	GLN	3.0
1	C	95	ASN	3.0
1	A	122	SER	2.9
1	C	130	ILE	2.9
1	D	220	THR	2.9
1	C	129	ASN	2.9
1	A	66	SER	2.9
1	C	193	ASN	2.9
1	E	217	ASN	2.8
1	C	101	VAL	2.8
1	D	169	PRO	2.8
1	E	232	ILE	2.8
1	G	66	SER	2.8
1	G	173	SER	2.8
1	F	64	LEU	2.8
1	G	172	GLY	2.8
1	C	167	ASN	2.8
1	G	224	SER	2.8
1	C	69	THR	2.8
1	C	89	LEU	2.8
1	G	128	ASN	2.7
1	C	219	VAL	2.7
1	F	114	GLY	2.7
1	H	174	LEU	2.7
1	F	118	GLY	2.7
1	B	69	THR	2.6
1	D	70	ASP	2.6
1	G	170	VAL	2.6
1	H	70	ASP	2.6
1	G	65	PRO	2.6
1	D	168	MET	2.6
1	E	277	LYS	2.6
1	D	218	GLY	2.6
1	G	107	GLY	2.6
1	C	177	LEU	2.6
1	C	166	VAL	2.6
1	D	219	VAL	2.6
1	E	65	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	125	PRO	2.5
1	B	173	SER	2.5
1	G	100	ASP	2.5
1	F	113	VAL	2.5
1	H	197	ILE	2.5
1	C	71	LEU	2.5
1	E	222	VAL	2.5
1	E	105	GLY	2.4
1	F	217	ASN	2.4
1	H	129	ASN	2.4
1	D	174	LEU	2.4
1	D	172	GLY	2.4
1	B	223	GLN	2.4
1	E	274	PHE	2.4
1	G	217	ASN	2.4
1	C	85	LEU	2.3
1	F	65	PRO	2.3
1	E	173	SER	2.3
1	C	83	GLY	2.3
1	A	223	GLN	2.3
1	E	127	LEU	2.3
1	F	221	PRO	2.3
1	A	65	PRO	2.3
1	C	201	LEU	2.2
1	H	239	GLU	2.2
1	H	222	VAL	2.2
1	F	195	GLY	2.2
1	H	194	GLN	2.2
1	F	117	LEU	2.2
1	A	222	VAL	2.2
1	A	277	LYS	2.2
1	C	84	LEU	2.2
1	A	104	SER	2.2
1	A	124	VAL	2.1
1	A	217	ASN	2.1
1	F	115	GLY	2.1
1	F	196	ARG	2.1
1	G	104	SER	2.1
1	A	195	GLY	2.1
1	G	106	GLY	2.1
1	C	196	ARG	2.1
1	C	131	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	220	THR	2.1
1	F	194	GLN	2.0
1	A	193	ASN	2.0
1	H	139	GLN	2.0
1	C	165	ASN	2.0
1	D	128	ASN	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 oligosaccharides 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
2	NA	D	301	1/1	0.51	0.20	78,78,78,78	0
2	NA	B	302	1/1	0.73	0.16	64,64,64,64	0
2	NA	F	304	1/1	0.73	0.16	67,67,67,67	0
4	GOL	H	301	6/6	0.78	0.16	45,58,68,70	0
4	GOL	C	301	6/6	0.79	0.18	47,58,72,72	0
2	NA	A	306	1/1	0.79	0.14	66,66,66,66	0
2	NA	H	307	1/1	0.80	0.10	75,75,75,75	0
2	NA	D	304	1/1	0.81	0.41	52,52,52,52	0
4	GOL	G	301	6/6	0.83	0.17	42,51,62,66	0
2	NA	E	307	1/1	0.83	0.12	62,62,62,62	0
4	GOL	H	302	6/6	0.83	0.16	44,62,75,75	0
2	NA	G	313	1/1	0.84	0.26	54,54,54,54	0
2	NA	D	303	1/1	0.85	0.13	68,68,68,68	0
3	CL	B	307	1/1	0.85	0.23	63,63,63,63	0
2	NA	A	305	1/1	0.86	0.10	47,47,47,47	0
2	NA	G	309	1/1	0.87	0.13	48,48,48,48	0
2	NA	D	302	1/1	0.87	0.17	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NA	C	305	1/1	0.88	0.10	58,58,58,58	0
2	NA	C	306	1/1	0.88	0.26	51,51,51,51	0
2	NA	C	302	1/1	0.88	0.12	51,51,51,51	0
2	NA	C	303	1/1	0.88	0.17	45,45,45,45	0
2	NA	H	308	1/1	0.89	0.15	65,65,65,65	0
2	NA	G	304	1/1	0.89	0.09	65,65,65,65	0
2	NA	G	310	1/1	0.89	0.13	55,55,55,55	0
2	NA	G	302	1/1	0.90	0.22	63,63,63,63	0
2	NA	F	302	1/1	0.90	0.14	49,49,49,49	0
2	NA	F	303	1/1	0.90	0.21	47,47,47,47	0
2	NA	E	301	1/1	0.90	0.19	39,39,39,39	0
2	NA	A	309	1/1	0.91	0.13	49,49,49,49	0
2	NA	B	303	1/1	0.91	0.09	46,46,46,46	0
2	NA	G	303	1/1	0.91	0.11	42,42,42,42	0
2	NA	B	304	1/1	0.91	0.11	36,36,36,36	0
2	NA	C	307	1/1	0.91	0.15	53,53,53,53	0
2	NA	B	306	1/1	0.91	0.11	46,46,46,46	0
2	NA	B	301	1/1	0.91	0.15	48,48,48,48	0
2	NA	G	311	1/1	0.92	0.13	57,57,57,57	0
2	NA	F	305	1/1	0.92	0.08	43,43,43,43	0
2	NA	G	314	1/1	0.92	0.09	46,46,46,46	0
2	NA	E	308	1/1	0.92	0.11	53,53,53,53	0
2	NA	E	309	1/1	0.92	0.08	42,42,42,42	0
2	NA	A	308	1/1	0.92	0.14	51,51,51,51	0
2	NA	G	306	1/1	0.92	0.10	55,55,55,55	0
2	NA	G	308	1/1	0.92	0.10	58,58,58,58	0
2	NA	E	305	1/1	0.92	0.15	51,51,51,51	0
2	NA	A	303	1/1	0.92	0.10	45,45,45,45	0
2	NA	A	304	1/1	0.93	0.07	45,45,45,45	0
2	NA	H	304	1/1	0.93	0.14	56,56,56,56	0
2	NA	G	307	1/1	0.93	0.15	51,51,51,51	0
2	NA	E	303	1/1	0.93	0.11	54,54,54,54	0
2	NA	F	301	1/1	0.93	0.06	41,41,41,41	0
2	NA	C	308	1/1	0.93	0.13	69,69,69,69	0
2	NA	A	301	1/1	0.93	0.22	49,49,49,49	0
2	NA	G	312	1/1	0.93	0.12	60,60,60,60	0
2	NA	G	305	1/1	0.93	0.12	43,43,43,43	0
2	NA	H	306	1/1	0.94	0.12	65,65,65,65	0
2	NA	C	304	1/1	0.94	0.12	57,57,57,57	0
2	NA	B	305	1/1	0.94	0.24	43,43,43,43	0
2	NA	E	302	1/1	0.94	0.07	49,49,49,49	0
2	NA	A	302	1/1	0.95	0.07	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NA	C	309	1/1	0.95	0.18	60,60,60,60	0
2	NA	A	310	1/1	0.95	0.13	44,44,44,44	0
2	NA	A	311	1/1	0.95	0.18	47,47,47,47	0
2	NA	E	304	1/1	0.96	0.06	48,48,48,48	0
2	NA	H	309	1/1	0.97	0.27	52,52,52,52	0
2	NA	H	305	1/1	0.97	0.05	41,41,41,41	0
2	NA	A	307	1/1	0.97	0.06	42,42,42,42	0
2	NA	H	303	1/1	0.98	0.05	36,36,36,36	0
2	NA	E	306	1/1	0.98	0.03	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.