



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:10 AM UTC

PDB ID : 4Q79 / pdb_00004q79
Title : Structure of a HG-derivative CsgG
Authors : Huang, Y.; Zhang, C.X.; Cao, B.; Zhao, Y.; Kou, Y.; Ni, D.
Deposited on : 2014-04-24
Resolution : 3.10 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:

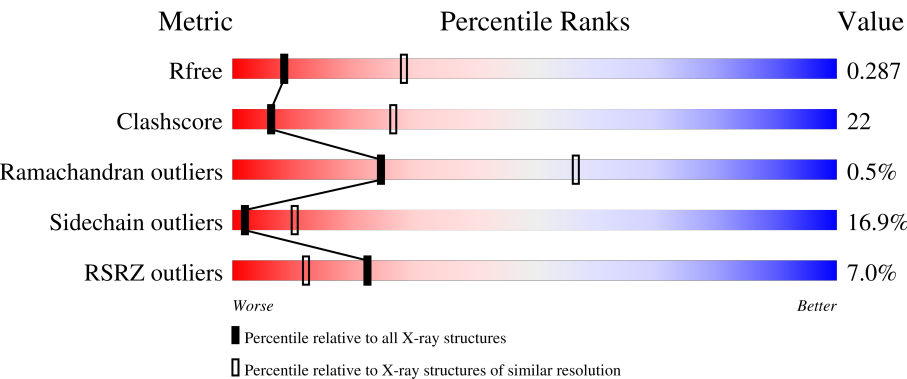
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	277	
1	B	277	
1	C	277	
1	D	277	
1	E	277	

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Mol	Chain	Length	Quality of chain
1	F	277	6% 35%27%6%32%
1	G	277	4% 33%32%31%
1	H	277	5% 35%28%6%31%
1	I	277	5% 36%27%6%31%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13035 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 CsgG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	189	Total	C	N	O	S	0	0	0
			1424	904	236	279	5			
1	A	196	Total	C	N	O	S	0	0	0
			1467	932	243	287	5			
1	B	190	Total	C	N	O	S	0	0	0
			1423	902	236	280	5			
1	C	198	Total	C	N	O	S	0	0	0
			1494	952	248	289	5			
1	E	198	Total	C	N	O	S	0	0	0
			1494	952	248	289	5			
1	F	189	Total	C	N	O	S	0	0	0
			1424	904	236	279	5			
1	G	190	Total	C	N	O	S	0	0	0
			1440	918	237	280	5			
1	H	191	Total	C	N	O	S	0	0	0
			1437	913	238	281	5			
1	I	190	Total	C	N	O	S	0	0	0
			1423	902	236	280	5			

- Molecule 2 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Hg	0	0
			1	1		
2	A	1	Total	Hg	0	0
			1	1		
2	B	1	Total	Hg	0	0
			1	1		
2	C	1	Total	Hg	0	0
			1	1		
2	E	1	Total	Hg	0	0
			1	1		

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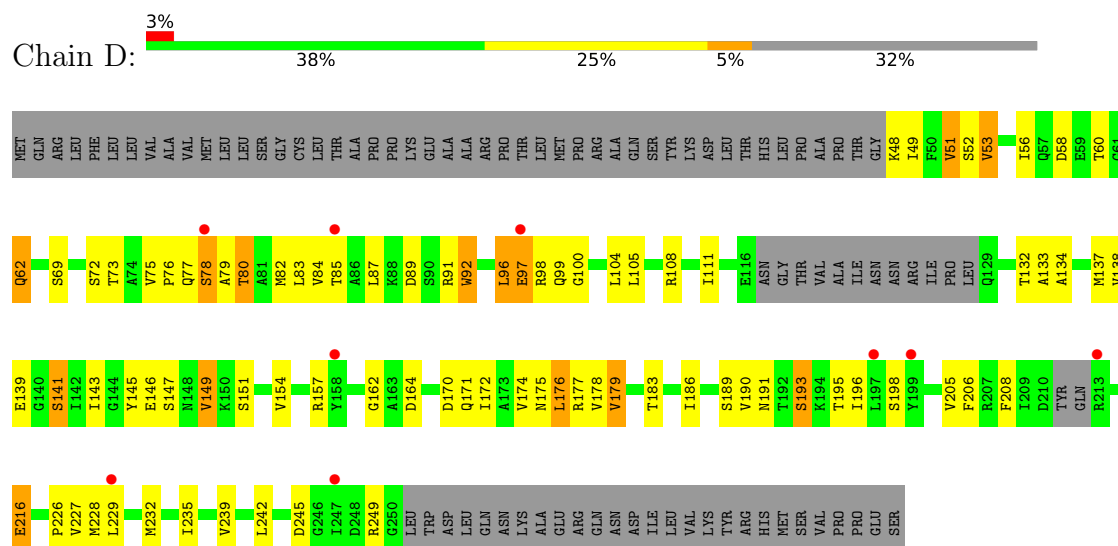
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	F	1	Total 1	Hg 1	0	0
2	G	1	Total 1	Hg 1	0	0
2	H	1	Total 1	Hg 1	0	0
2	I	1	Total 1	Hg 1	0	0

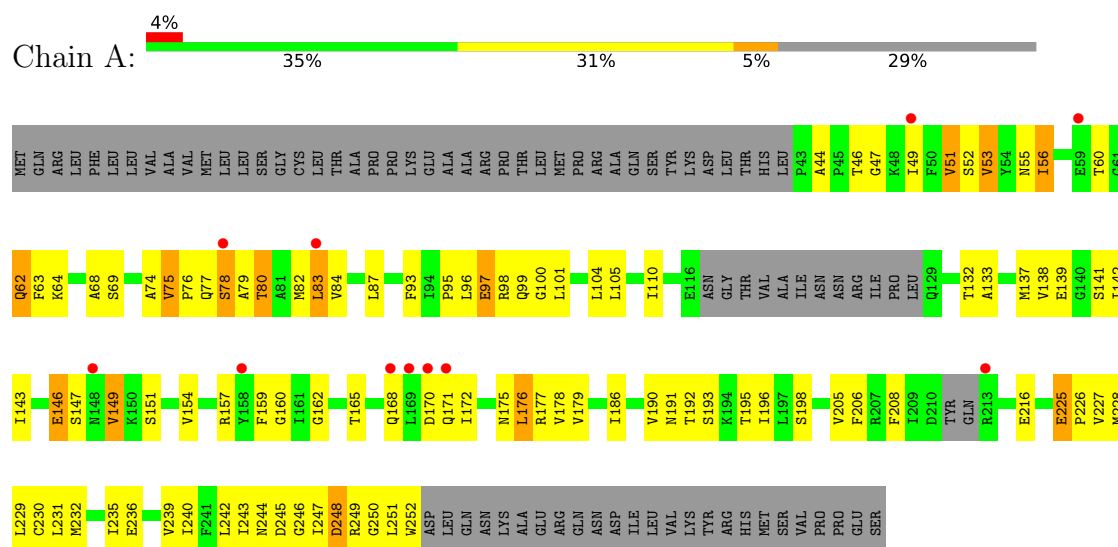
3 Residue-property plots [i](#)

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 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: CsgG

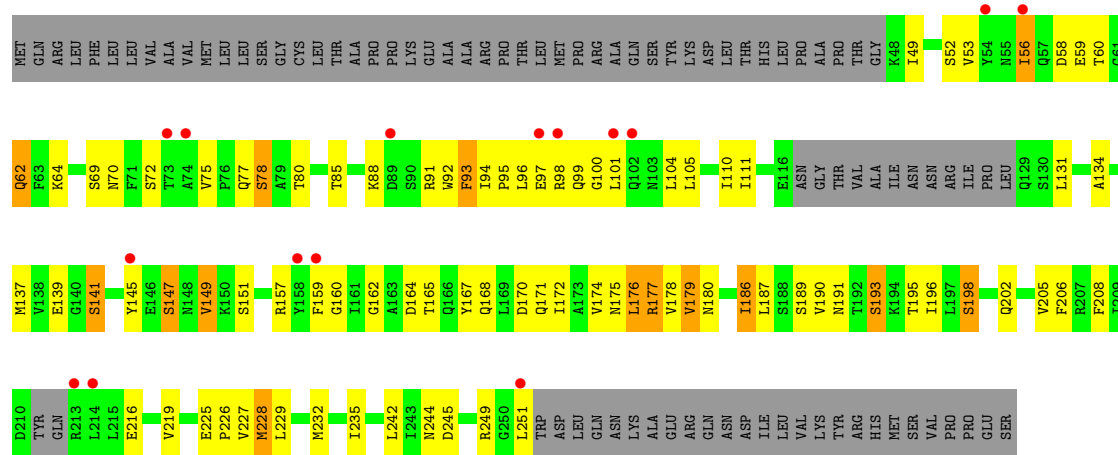


• Molecule 1: CsgG

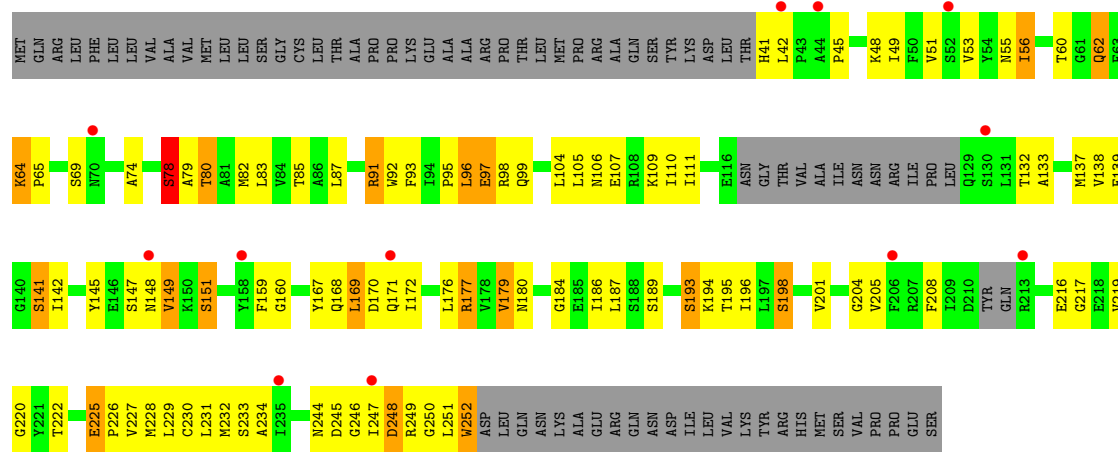


• Molecule 1: CsgG

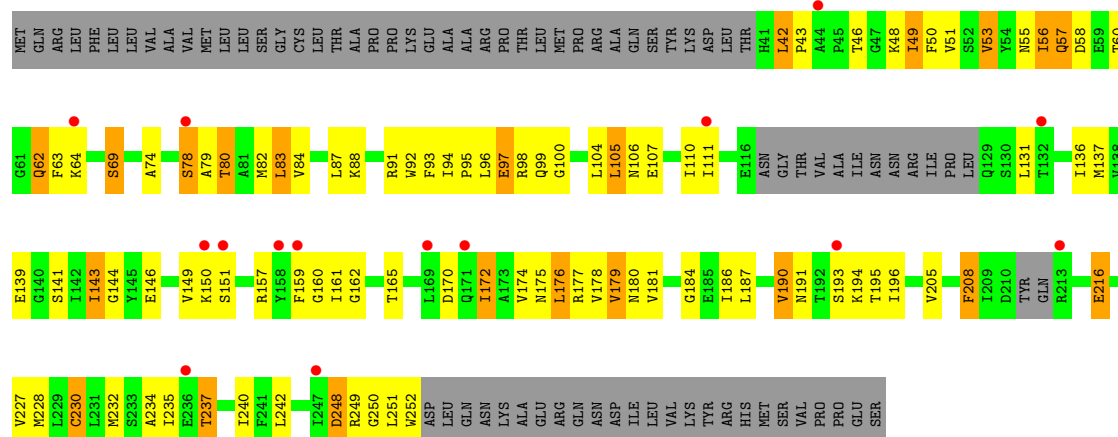




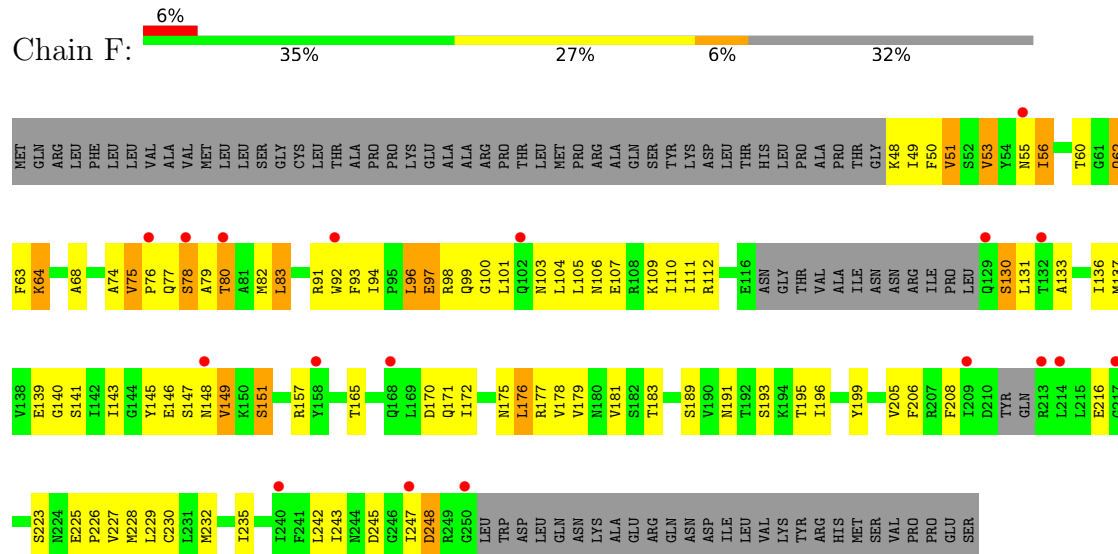
• Molecule 1: CsgG



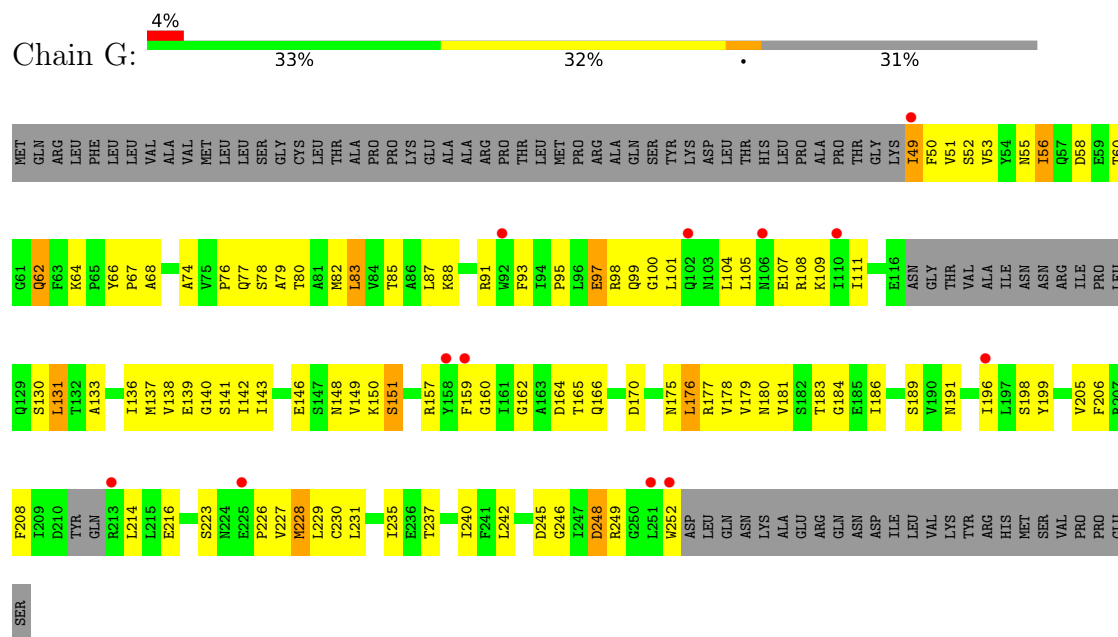
• Molecule 1: CsgG



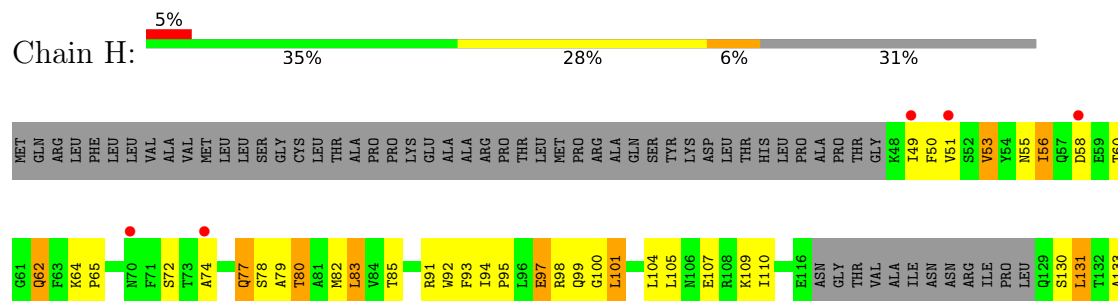
• Molecule 1: CsgG

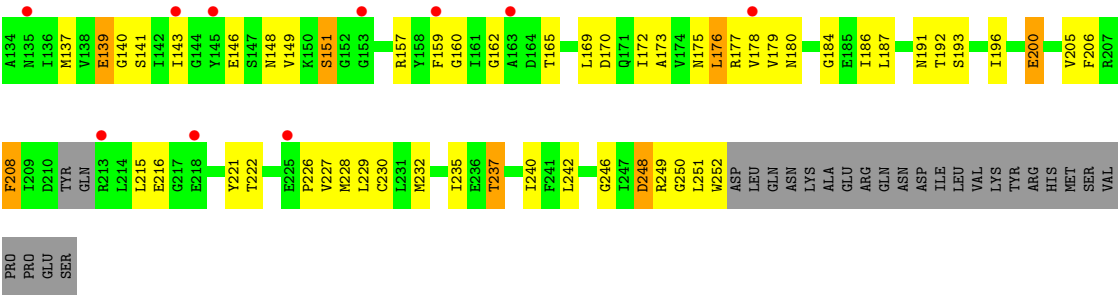


• Molecule 1: CsgG

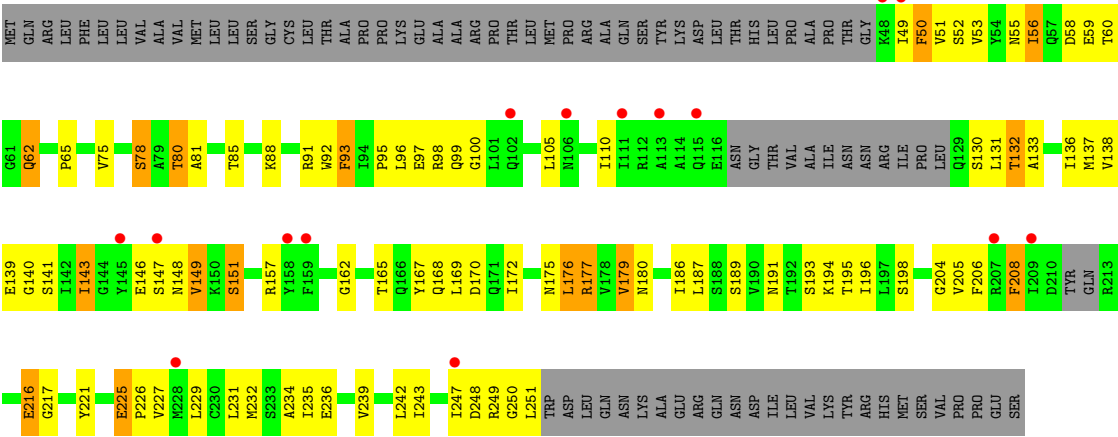


• Molecule 1: CsgG





● Molecule 1: CsgG



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	171.64Å 176.88Å 104.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.25 – 3.10 49.25 – 3.10	Depositor EDS
% Data completeness (in resolution range)	58.3 (49.25-3.10) 59.4 (49.25-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 3.07Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.236 , 0.278 0.259 , 0.287	Depositor DCC
R_{free} test set	1760 reflections (4.12%)	wwPDB-VP
Wilson B-factor (Å ²)	82.4	Xtriage
Anisotropy	1.384	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 92.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.045 for k,h,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	13035	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 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: HG

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	0/1488	0.93	4/2019 (0.2%)
1	B	0.41	0/1440	0.89	0/1951
1	C	0.44	0/1518	0.95	3/2062 (0.1%)
1	D	0.41	0/1443	0.90	0/1956
1	E	0.41	0/1518	0.92	1/2062 (0.0%)
1	F	0.40	0/1443	0.89	2/1956 (0.1%)
1	G	0.39	0/1461	0.90	0/1983
1	H	0.40	0/1456	0.87	0/1974
1	I	0.40	0/1440	0.91	3/1951 (0.2%)
All	All	0.41	0/13207	0.91	13/17914 (0.1%)

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	C	0	1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	225	GLU	CA-C-N	6.66	128.16	119.84
1	I	225	GLU	C-N-CA	6.66	128.16	119.84
1	A	44	ALA	CA-C-N	5.99	127.33	119.84
1	A	44	ALA	C-N-CA	5.99	127.33	119.84
1	C	225	GLU	CA-C-N	5.99	127.33	119.84
1	C	225	GLU	C-N-CA	5.99	127.33	119.84
1	A	225	GLU	CA-C-N	5.89	127.20	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	GLU	C-N-CA	5.89	127.20	119.84
1	F	225	GLU	CA-C-N	5.33	126.50	119.84
1	F	225	GLU	C-N-CA	5.33	126.50	119.84
1	E	144	GLY	N-CA-C	5.15	118.21	110.18
1	I	143	ILE	N-CA-C	5.14	115.81	110.82
1	C	78	SER	N-CA-C	5.05	119.20	113.19

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	91	ARG	Peptide

5.2 Too-close contacts ⓘ

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	1467	0	1450	79	0
1	B	1423	0	1410	65	0
1	C	1494	0	1475	86	0
1	D	1424	0	1407	73	0
1	E	1494	0	1475	79	0
1	F	1424	0	1407	78	0
1	G	1440	0	1424	71	0
1	H	1437	0	1420	76	0
1	I	1423	0	1410	60	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
All	All	13035	0	12878	570	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 22.

All (570) 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:G:177:ARG:NH1	1:I:97:GLU:OE2	2.04	0.90
1:G:98:ARG:HG3	1:G:101:LEU:HD12	1.55	0.85
1:F:97:GLU:OE2	1:H:177:ARG:NH1	2.10	0.84
1:H:56:ILE:HG13	1:H:141:SER:HA	1.59	0.83
1:G:170:ASP:HB2	1:G:196:ILE:HB	1.61	0.83
1:F:170:ASP:HB2	1:F:196:ILE:HB	1.62	0.81
1:F:205:VAL:O	1:F:216:GLU:HA	1.81	0.80
1:C:56:ILE:HG13	1:C:141:SER:HA	1.63	0.80
1:E:60:THR:HG23	1:E:62:GLN:H	1.47	0.79
1:A:196:ILE:HD13	1:A:227:VAL:HG22	1.65	0.79
1:E:175:ASN:ND2	1:E:191:ASN:OD1	2.15	0.79
1:E:177:ARG:NH1	1:H:97:GLU:OE2	2.17	0.78
1:C:205:VAL:O	1:C:216:GLU:HA	1.83	0.77
1:I:60:THR:HG23	1:I:62:GLN:H	1.48	0.77
1:I:205:VAL:O	1:I:216:GLU:HA	1.84	0.77
1:A:186:ILE:HD12	1:B:95:PRO:HB2	1.67	0.77
1:F:196:ILE:HD13	1:F:227:VAL:HG22	1.67	0.76
1:C:194:LYS:HE3	1:C:234:ALA:HA	1.68	0.75
1:A:56:ILE:HG22	1:A:80:THR:HG23	1.68	0.75
1:G:56:ILE:HG13	1:G:141:SER:HA	1.69	0.74
1:D:56:ILE:HG13	1:D:141:SER:HA	1.70	0.74
1:D:56:ILE:HG22	1:D:80:THR:HG23	1.70	0.74
1:B:196:ILE:HD13	1:B:227:VAL:HG22	1.68	0.74
1:E:56:ILE:HG13	1:E:141:SER:HA	1.70	0.73
1:I:143:ILE:HD11	1:I:175:ASN:HB2	1.70	0.73
1:D:186:ILE:HD12	1:C:95:PRO:HB2	1.70	0.73
1:H:205:VAL:O	1:H:216:GLU:HA	1.89	0.73
1:D:170:ASP:HB2	1:D:196:ILE:HB	1.72	0.72
1:G:237:THR:HA	1:G:240:ILE:HD12	1.72	0.72
1:B:205:VAL:O	1:B:216:GLU:HA	1.91	0.71
1:A:205:VAL:O	1:A:216:GLU:HA	1.91	0.71
1:H:175:ASN:ND2	1:H:191:ASN:OD1	2.23	0.70
1:C:137:MET:HB3	1:C:179:VAL:HG13	1.72	0.70
1:A:53:VAL:HG21	1:A:83:LEU:HD12	1.74	0.70
1:A:62:GLN:OE1	1:B:64:LYS:NZ	2.25	0.70
1:H:148:ASN:HB3	1:H:151:SER:HB3	1.74	0.70
1:D:82:MET:HE2	1:D:232:MET:HE2	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:56:ILE:HG22	1:G:80:THR:HG23	1.74	0.69
1:F:103:ASN:ND2	1:H:139:GLU:OE2	2.26	0.69
1:D:196:ILE:HD13	1:D:227:VAL:HG22	1.74	0.69
1:D:48:LYS:HA	1:D:92:TRP:HB3	1.73	0.69
1:B:137:MET:HE1	1:E:104:LEU:HA	1.73	0.69
1:A:170:ASP:HB2	1:A:196:ILE:HB	1.74	0.69
1:I:170:ASP:HB2	1:I:196:ILE:HB	1.74	0.69
1:C:170:ASP:O	1:C:195:THR:HA	1.93	0.68
1:G:175:ASN:ND2	1:G:191:ASN:OD1	2.26	0.68
1:A:56:ILE:HG13	1:A:141:SER:HA	1.75	0.68
1:D:97:GLU:OE2	1:F:177:ARG:NH1	2.28	0.67
1:E:175:ASN:HD21	1:H:85:THR:HG21	1.58	0.67
1:H:53:VAL:HG21	1:H:83:LEU:HD12	1.76	0.67
1:D:137:MET:HE1	1:C:104:LEU:HA	1.76	0.67
1:I:176:LEU:HB3	1:I:242:LEU:HD11	1.76	0.67
1:G:76:PRO:HG2	1:G:228:MET:HB2	1.77	0.67
1:A:172:ILE:HD11	1:A:227:VAL:HG13	1.78	0.66
1:G:228:MET:HE3	1:G:229:LEU:HG	1.77	0.66
1:D:78:SER:OG	1:F:143:ILE:O	2.13	0.66
1:F:56:ILE:HG13	1:F:141:SER:HA	1.76	0.66
1:G:196:ILE:HD13	1:G:227:VAL:HG22	1.77	0.66
1:C:245:ASP:HB3	1:C:249:ARG:HH21	1.60	0.66
1:F:110:ILE:HG22	1:H:133:ALA:HB2	1.78	0.66
1:H:82:MET:HE2	1:H:232:MET:HE2	1.77	0.66
1:F:226:PRO:HB2	1:F:229:LEU:HB2	1.78	0.65
1:H:170:ASP:HB2	1:H:196:ILE:HB	1.78	0.65
1:I:157:ARG:HH22	1:I:206:PHE:HB2	1.61	0.65
1:I:172:ILE:HD11	1:I:227:VAL:HG13	1.77	0.65
1:H:176:LEU:HB3	1:H:242:LEU:HD11	1.79	0.65
1:G:140:GLY:HA3	1:G:175:ASN:O	1.96	0.65
1:B:177:ARG:NH1	1:E:97:GLU:OE2	2.30	0.65
1:E:205:VAL:O	1:E:216:GLU:HA	1.97	0.64
1:I:175:ASN:ND2	1:I:191:ASN:OD1	2.27	0.64
1:A:97:GLU:OE2	1:I:177:ARG:NH1	2.30	0.64
1:C:169:LEU:HA	1:C:196:ILE:O	1.96	0.64
1:G:55:ASN:HA	1:G:80:THR:HG21	1.79	0.64
1:G:205:VAL:O	1:G:216:GLU:HA	1.97	0.64
1:F:104:LEU:HA	1:H:137:MET:HE1	1.78	0.64
1:H:157:ARG:HH22	1:H:206:PHE:HB2	1.62	0.64
1:D:172:ILE:HG13	1:D:196:ILE:HD11	1.80	0.64
1:C:137:MET:HE1	1:G:104:LEU:HA	1.78	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:GLN:HG2	1:C:195:THR:HG22	1.80	0.63
1:D:245:ASP:HB3	1:D:249:ARG:HH21	1.64	0.63
1:H:237:THR:HA	1:H:240:ILE:HD12	1.81	0.63
1:E:98:ARG:NH1	1:H:107:GLU:OE1	2.32	0.62
1:B:137:MET:HB3	1:B:179:VAL:HG13	1.80	0.62
1:D:104:LEU:HA	1:F:137:MET:HE1	1.81	0.62
1:G:164:ASP:OD2	1:G:166:GLN:NE2	2.33	0.62
1:G:176:LEU:HB3	1:G:242:LEU:HD11	1.81	0.62
1:D:147:SER:HA	1:D:149:VAL:HG23	1.81	0.62
1:D:205:VAL:O	1:D:216:GLU:HA	1.99	0.62
1:E:48:LYS:HG2	1:E:92:TRP:HB2	1.80	0.62
1:C:194:LYS:NZ	1:C:233:SER:OG	2.32	0.62
1:B:56:ILE:HG13	1:B:141:SER:HA	1.82	0.61
1:A:172:ILE:HG13	1:A:196:ILE:HD11	1.83	0.61
1:F:143:ILE:HD11	1:F:175:ASN:HB2	1.81	0.61
1:I:180:ASN:HB2	1:I:187:LEU:HD11	1.83	0.61
1:D:137:MET:HB3	1:D:179:VAL:HG13	1.81	0.61
1:D:172:ILE:HD11	1:D:227:VAL:HG13	1.83	0.61
1:D:99:GLN:HG2	1:F:177:ARG:HH22	1.66	0.61
1:E:55:ASN:HB3	1:E:57:GLN:HE21	1.63	0.61
1:A:157:ARG:HH22	1:A:206:PHE:HB2	1.65	0.60
1:C:56:ILE:HG22	1:C:80:THR:HG23	1.82	0.60
1:E:92:TRP:HE3	1:E:92:TRP:H	1.48	0.60
1:C:53:VAL:HG21	1:C:83:LEU:HD12	1.82	0.60
1:B:178:VAL:HG23	1:B:242:LEU:HD22	1.82	0.60
1:C:64:LYS:HG2	1:C:74:ALA:HA	1.83	0.60
1:G:49:ILE:HB	1:G:252:TRP:HZ3	1.65	0.60
1:H:60:THR:HG23	1:H:62:GLN:H	1.65	0.60
1:E:56:ILE:HG22	1:E:80:THR:HG23	1.84	0.59
1:D:149:VAL:HG13	1:C:226:PRO:HG3	1.83	0.59
1:A:64:LYS:NZ	1:I:62:GLN:OE1	2.34	0.59
1:G:98:ARG:NH2	1:I:110:ILE:HD13	2.17	0.59
1:B:176:LEU:HB3	1:B:242:LEU:HD11	1.84	0.59
1:F:226:PRO:HG2	1:F:229:LEU:HD12	1.84	0.59
1:E:248:ASP:N	1:E:248:ASP:OD1	2.36	0.59
1:A:249:ARG:H	1:A:250:GLY:HA2	1.67	0.59
1:B:172:ILE:HD11	1:B:227:VAL:HG13	1.83	0.59
1:D:172:ILE:O	1:D:193:SER:HA	2.02	0.59
1:G:79:ALA:O	1:G:80:THR:OG1	2.18	0.59
1:D:62:GLN:OE1	1:C:64:LYS:NZ	2.32	0.58
1:C:51:VAL:HG11	1:C:87:LEU:HD13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:LYS:HG2	1:C:92:TRP:HB2	1.84	0.58
1:H:79:ALA:O	1:H:80:THR:OG1	2.18	0.58
1:C:147:SER:HB2	1:C:148:ASN:HA	1.85	0.58
1:C:177:ARG:NH1	1:G:97:GLU:OE2	2.37	0.58
1:A:143:ILE:O	1:B:78:SER:OG	2.15	0.58
1:F:172:ILE:HD11	1:F:227:VAL:HG13	1.86	0.58
1:D:60:THR:HG23	1:D:62:GLN:HB2	1.85	0.58
1:D:177:ARG:HH22	1:C:99:GLN:HG2	1.67	0.58
1:D:53:VAL:HG21	1:D:83:LEU:HD12	1.86	0.58
1:G:64:LYS:HG2	1:G:74:ALA:HA	1.85	0.58
1:F:48:LYS:HD3	1:F:94:ILE:HD11	1.86	0.57
1:F:178:VAL:HG23	1:F:242:LEU:HD22	1.86	0.57
1:H:173:ALA:HA	1:H:192:THR:O	2.04	0.57
1:A:248:ASP:OD1	1:A:248:ASP:N	2.37	0.57
1:E:137:MET:HE1	1:H:104:LEU:HA	1.86	0.57
1:E:170:ASP:O	1:E:195:THR:HA	2.04	0.57
1:G:248:ASP:N	1:G:248:ASP:OD1	2.38	0.57
1:C:149:VAL:HG11	1:C:171:GLN:HG3	1.85	0.57
1:B:228:MET:HE3	1:B:229:LEU:HG	1.87	0.57
1:E:79:ALA:O	1:E:80:THR:OG1	2.19	0.57
1:F:149:VAL:HG21	1:F:171:GLN:HG3	1.87	0.57
1:B:170:ASP:HB2	1:B:196:ILE:HB	1.87	0.56
1:A:68:ALA:HA	1:I:65:PRO:HB3	1.88	0.56
1:A:99:GLN:HG2	1:I:177:ARG:HH22	1.71	0.56
1:C:170:ASP:HB2	1:C:196:ILE:HB	1.86	0.56
1:E:143:ILE:HG12	1:H:78:SER:HB2	1.87	0.56
1:H:143:ILE:HD11	1:H:175:ASN:HB2	1.86	0.56
1:A:143:ILE:HD11	1:A:175:ASN:HB2	1.87	0.56
1:E:161:ILE:HG13	1:E:205:VAL:HG22	1.88	0.56
1:G:148:ASN:HB3	1:G:151:SER:HB3	1.88	0.56
1:I:140:GLY:HA3	1:I:175:ASN:O	2.06	0.56
1:B:98:ARG:NH2	1:E:110:ILE:HD13	2.21	0.55
1:C:167:TYR:HA	1:C:198:SER:O	2.07	0.55
1:D:53:VAL:HG22	1:D:80:THR:HG22	1.87	0.55
1:F:60:THR:HG23	1:F:62:GLN:H	1.72	0.55
1:A:46:THR:HB	1:A:47:GLY:HA3	1.87	0.55
1:B:180:ASN:HB2	1:B:187:LEU:HD11	1.87	0.55
1:E:179:VAL:HB	1:E:186:ILE:HG12	1.88	0.55
1:H:55:ASN:HA	1:H:80:THR:HG21	1.89	0.55
1:A:55:ASN:HA	1:A:80:THR:HG21	1.89	0.55
1:A:147:SER:HA	1:A:149:VAL:HG23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:ASN:HA	1:E:69:SER:HB2	1.89	0.55
1:C:133:ALA:HB1	1:G:111:ILE:HG12	1.87	0.55
1:H:200:GLU:HB3	1:H:222:THR:HG22	1.89	0.55
1:D:175:ASN:ND2	1:D:191:ASN:OD1	2.30	0.54
1:B:157:ARG:HH22	1:B:206:PHE:HB2	1.72	0.54
1:D:99:GLN:HB3	1:D:100:GLY:HA3	1.88	0.54
1:D:151:SER:OG	1:C:222:THR:OG1	2.24	0.54
1:A:249:ARG:N	1:A:250:GLY:HA2	2.22	0.54
1:C:179:VAL:HG21	1:G:97:GLU:HG3	1.89	0.54
1:D:176:LEU:HB3	1:D:242:LEU:HD11	1.88	0.54
1:G:157:ARG:HH22	1:G:206:PHE:HB2	1.72	0.54
1:D:73:THR:HG21	1:D:77:GLN:HE22	1.72	0.54
1:B:98:ARG:HG3	1:B:101:LEU:HD12	1.89	0.54
1:F:48:LYS:HA	1:F:92:TRP:HB2	1.89	0.54
1:G:82:MET:HB3	1:G:235:ILE:HG21	1.89	0.54
1:I:226:PRO:HB2	1:I:229:LEU:HG	1.89	0.54
1:D:79:ALA:O	1:D:80:THR:OG1	2.21	0.54
1:D:154:VAL:HG12	1:C:219:VAL:HG12	1.89	0.54
1:E:150:LYS:HG3	1:H:221:TYR:HE1	1.73	0.54
1:E:170:ASP:HB2	1:E:196:ILE:HB	1.90	0.54
1:E:237:THR:HA	1:E:240:ILE:HD12	1.90	0.53
1:F:110:ILE:HD13	1:H:98:ARG:NH2	2.23	0.53
1:B:172:ILE:HG13	1:B:196:ILE:HD11	1.90	0.53
1:H:226:PRO:HB2	1:H:229:LEU:HB2	1.91	0.53
1:F:107:GLU:CD	1:H:98:ARG:HH12	2.16	0.53
1:A:226:PRO:O	1:A:229:LEU:N	2.39	0.53
1:D:111:ILE:HG12	1:F:133:ALA:HB1	1.89	0.53
1:E:175:ASN:ND2	1:H:85:THR:HG21	2.23	0.53
1:H:248:ASP:OD1	1:H:248:ASP:N	2.42	0.53
1:E:64:LYS:HD3	1:E:74:ALA:HA	1.91	0.53
1:G:150:LYS:HG3	1:I:221:TYR:HE1	1.74	0.53
1:B:60:THR:OG1	1:B:145:TYR:N	2.42	0.53
1:B:174:VAL:O	1:B:191:ASN:HA	2.08	0.52
1:F:97:GLU:HG2	1:H:186:ILE:HG12	1.91	0.52
1:H:196:ILE:HD13	1:H:227:VAL:HG22	1.90	0.52
1:C:92:TRP:H	1:C:92:TRP:HE3	1.56	0.52
1:H:56:ILE:HG22	1:H:80:THR:HG23	1.92	0.52
1:I:98:ARG:NH2	1:I:132:THR:O	2.42	0.52
1:E:180:ASN:HB2	1:E:187:LEU:HD11	1.91	0.52
1:E:196:ILE:HG12	1:E:230:CYS:SG	2.49	0.52
1:D:53:VAL:HG11	1:D:84:VAL:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:MET:HE1	1:B:104:LEU:HA	1.92	0.52
1:B:186:ILE:HD11	1:E:97:GLU:HA	1.90	0.52
1:C:45:PRO:HG3	1:C:92:TRP:CZ2	2.44	0.52
1:F:110:ILE:HG21	1:H:98:ARG:NH2	2.24	0.52
1:F:175:ASN:ND2	1:F:191:ASN:OD1	2.43	0.52
1:H:60:THR:O	1:H:62:GLN:NE2	2.42	0.52
1:G:60:THR:HG23	1:G:62:GLN:H	1.75	0.52
1:I:88:LYS:HB2	1:I:95:PRO:HG2	1.90	0.52
1:C:145:TYR:OH	1:C:170:ASP:OD2	2.15	0.51
1:F:137:MET:HE3	1:F:181:VAL:HG22	1.93	0.51
1:I:151:SER:HB2	1:I:168:GLN:HA	1.91	0.51
1:F:104:LEU:HD11	1:H:184:GLY:HA2	1.92	0.51
1:A:133:ALA:HB1	1:B:111:ILE:HG12	1.93	0.51
1:C:151:SER:HB2	1:C:168:GLN:HA	1.92	0.51
1:C:177:ARG:HG2	1:C:189:SER:HB2	1.92	0.51
1:F:226:PRO:O	1:F:229:LEU:N	2.41	0.51
1:D:171:GLN:HG2	1:D:195:THR:HG22	1.92	0.51
1:D:174:VAL:O	1:D:191:ASN:HA	2.11	0.51
1:A:244:ASN:HA	1:A:247:ILE:HB	1.92	0.51
1:B:58:ASP:OD1	1:B:60:THR:HG22	2.10	0.51
1:C:189:SER:OG	1:G:85:THR:HG22	2.11	0.51
1:G:143:ILE:O	1:I:78:SER:OG	2.23	0.51
1:A:110:ILE:HG22	1:I:133:ALA:HB2	1.93	0.51
1:I:232:MET:HA	1:I:235:ILE:HG22	1.91	0.51
1:D:133:ALA:HB1	1:C:111:ILE:HG12	1.92	0.51
1:H:226:PRO:O	1:H:229:LEU:N	2.42	0.51
1:E:99:GLN:HB3	1:E:100:GLY:HA3	1.91	0.51
1:C:79:ALA:O	1:C:80:THR:OG1	2.26	0.51
1:E:84:VAL:HG13	1:E:95:PRO:HB3	1.93	0.51
1:A:63:PHE:H	1:B:72:SER:HB3	1.76	0.50
1:G:246:GLY:O	1:G:252:TRP:NE1	2.42	0.50
1:I:88:LYS:HD3	1:I:95:PRO:HD2	1.93	0.50
1:D:52:SER:HB2	1:D:134:ALA:HB3	1.92	0.50
1:H:140:GLY:HA3	1:H:175:ASN:O	2.11	0.50
1:A:177:ARG:NH1	1:B:97:GLU:OE2	2.44	0.50
1:A:239:VAL:O	1:A:243:ILE:HG13	2.12	0.50
1:E:83:LEU:HD23	1:E:235:ILE:HD11	1.94	0.50
1:F:56:ILE:HG22	1:F:80:THR:HG23	1.94	0.50
1:E:137:MET:HE3	1:E:181:VAL:HG22	1.92	0.50
1:B:98:ARG:NH1	1:E:107:GLU:OE1	2.45	0.50
1:B:149:VAL:HG11	1:B:171:GLN:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:ASP:OD1	1:C:248:ASP:N	2.43	0.50
1:C:201:VAL:O	1:C:220:GLY:HA2	2.11	0.50
1:F:145:TYR:HA	1:F:171:GLN:O	2.12	0.50
1:B:177:ARG:HB3	1:B:189:SER:HB3	1.93	0.50
1:F:79:ALA:O	1:F:80:THR:OG1	2.27	0.50
1:D:183:THR:HB	1:C:132:THR:HG23	1.92	0.49
1:A:87:LEU:O	1:A:93:PHE:HB2	2.12	0.49
1:C:82:MET:HE2	1:C:232:MET:HE2	1.92	0.49
1:C:249:ARG:HB3	1:C:250:GLY:C	2.37	0.49
1:C:106:ASN:OD1	1:C:109:LYS:NZ	2.45	0.49
1:C:193:SER:O	1:C:193:SER:OG	2.27	0.49
1:A:142:ILE:HD13	1:A:231:LEU:HD11	1.95	0.49
1:A:149:VAL:HG13	1:B:226:PRO:HG3	1.94	0.49
1:F:243:ILE:O	1:F:247:ILE:HG13	2.12	0.49
1:I:52:SER:O	1:I:137:MET:HG3	2.12	0.49
1:H:172:ILE:O	1:H:193:SER:HA	2.12	0.49
1:B:167:TYR:HA	1:B:198:SER:O	2.13	0.49
1:D:226:PRO:O	1:D:229:LEU:N	2.45	0.49
1:F:232:MET:HA	1:F:235:ILE:HG22	1.95	0.49
1:D:58:ASP:OD1	1:D:60:THR:HG22	2.13	0.49
1:D:98:ARG:NH2	1:C:110:ILE:HG21	2.28	0.48
1:B:98:ARG:HH22	1:E:110:ILE:HG21	1.78	0.48
1:F:97:GLU:HB3	1:F:98:ARG:H	1.53	0.48
1:G:143:ILE:HD11	1:G:175:ASN:HB2	1.94	0.48
1:G:226:PRO:O	1:G:229:LEU:N	2.45	0.48
1:D:91:ARG:HA	1:D:92:TRP:C	2.37	0.48
1:H:50:PHE:HD1	1:H:94:ILE:HB	1.79	0.48
1:A:191:ASN:OD1	1:B:85:THR:HG21	2.13	0.48
1:F:107:GLU:HA	1:F:110:ILE:HD12	1.94	0.48
1:G:99:GLN:HB3	1:G:100:GLY:HA3	1.95	0.48
1:G:245:ASP:HB3	1:G:249:ARG:HH21	1.78	0.48
1:A:60:THR:HG23	1:A:62:GLN:HB2	1.95	0.48
1:A:99:GLN:HB3	1:A:100:GLY:HA3	1.96	0.48
1:C:225:GLU:HA	1:C:226:PRO:HD3	1.68	0.48
1:C:246:GLY:O	1:C:250:GLY:HA2	2.12	0.48
1:G:52:SER:O	1:G:137:MET:HG3	2.13	0.48
1:G:133:ALA:HB2	1:I:110:ILE:HG22	1.96	0.48
1:A:79:ALA:O	1:A:80:THR:OG1	2.27	0.48
1:B:232:MET:HA	1:B:235:ILE:HG22	1.95	0.48
1:F:176:LEU:HB3	1:F:242:LEU:HD11	1.95	0.48
1:H:107:GLU:HA	1:H:110:ILE:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:ASN:HA	1:C:80:THR:HG21	1.94	0.48
1:C:252:TRP:H	1:C:252:TRP:CD1	2.31	0.48
1:H:226:PRO:HG2	1:H:229:LEU:HD12	1.95	0.48
1:A:196:ILE:HG12	1:A:230:CYS:SG	2.53	0.48
1:E:91:ARG:HA	1:E:93:PHE:N	2.29	0.48
1:E:98:ARG:NH2	1:H:110:ILE:HD13	2.29	0.48
1:F:99:GLN:HB3	1:F:100:GLY:HA3	1.96	0.48
1:D:245:ASP:O	1:D:249:ARG:HB2	2.14	0.47
1:D:96:LEU:HD12	1:D:98:ARG:NH1	2.28	0.47
1:D:177:ARG:NH1	1:C:97:GLU:OE2	2.47	0.47
1:C:244:ASN:O	1:C:247:ILE:HB	2.14	0.47
1:F:60:THR:HG23	1:F:62:GLN:N	2.30	0.47
1:G:83:LEU:HB2	1:G:235:ILE:HD11	1.96	0.47
1:E:98:ARG:HH12	1:H:107:GLU:CD	2.21	0.47
1:F:64:LYS:HD3	1:F:74:ALA:HA	1.94	0.47
1:D:143:ILE:O	1:C:78:SER:OG	2.20	0.47
1:I:147:SER:HA	1:I:149:VAL:HG23	1.96	0.47
1:A:151:SER:HB2	1:A:168:GLN:HG2	1.97	0.47
1:A:243:ILE:O	1:A:247:ILE:N	2.46	0.47
1:A:178:VAL:HG23	1:A:242:LEU:HD13	1.96	0.47
1:C:60:THR:OG1	1:C:145:TYR:N	2.47	0.47
1:F:98:ARG:HG3	1:F:101:LEU:HD12	1.95	0.47
1:E:55:ASN:HA	1:E:80:THR:HG21	1.96	0.47
1:E:82:MET:HE2	1:E:232:MET:HE2	1.95	0.47
1:F:78:SER:HB2	1:F:82:MET:SD	2.55	0.47
1:C:51:VAL:HG13	1:C:95:PRO:HA	1.97	0.47
1:C:91:ARG:HA	1:C:93:PHE:N	2.29	0.47
1:C:179:VAL:HA	1:C:186:ILE:HA	1.97	0.47
1:F:53:VAL:HG21	1:F:83:LEU:HD12	1.97	0.47
1:A:250:GLY:C	1:A:252:TRP:H	2.23	0.47
1:E:175:ASN:HA	1:E:190:VAL:O	2.15	0.47
1:G:137:MET:HE3	1:G:137:MET:HB2	1.67	0.47
1:I:99:GLN:HB3	1:I:100:GLY:HA3	1.97	0.47
1:I:235:ILE:O	1:I:239:VAL:HG23	2.15	0.47
1:A:64:LYS:HD3	1:A:74:ALA:HA	1.97	0.46
1:G:138:VAL:HG22	1:G:178:VAL:HG22	1.97	0.46
1:H:250:GLY:C	1:H:252:TRP:H	2.24	0.46
1:E:97:GLU:HB3	1:E:98:ARG:H	1.53	0.46
1:G:60:THR:HG23	1:G:62:GLN:N	2.29	0.46
1:B:245:ASP:HB3	1:B:249:ARG:HH21	1.80	0.46
1:B:147:SER:HA	1:B:149:VAL:HG23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:ILE:HD11	1:C:196:ILE:HD11	1.97	0.46
1:D:138:VAL:HG22	1:D:178:VAL:HG22	1.98	0.46
1:C:97:GLU:HB3	1:C:98:ARG:H	1.53	0.46
1:F:55:ASN:HA	1:F:80:THR:HG21	1.97	0.46
1:F:149:VAL:HG11	1:F:171:GLN:HG3	1.97	0.46
1:D:235:ILE:O	1:D:239:VAL:HG23	2.15	0.46
1:A:51:VAL:HG21	1:A:87:LEU:HD13	1.98	0.46
1:A:84:VAL:HG13	1:A:95:PRO:HB3	1.97	0.46
1:B:91:ARG:HA	1:B:93:PHE:N	2.30	0.46
1:B:97:GLU:HB3	1:B:98:ARG:H	1.53	0.46
1:G:177:ARG:HG2	1:G:189:SER:HB2	1.97	0.46
1:G:199:TYR:CZ	1:G:223:SER:HB3	2.50	0.46
1:H:159:PHE:HA	1:H:160:GLY:HA2	1.51	0.46
1:I:55:ASN:HA	1:I:80:THR:HG21	1.98	0.46
1:B:60:THR:HG23	1:B:62:GLN:HB2	1.96	0.46
1:B:164:ASP:OD1	1:B:202:GLN:HB2	2.16	0.46
1:B:171:GLN:HG2	1:B:195:THR:HG22	1.98	0.46
1:G:91:ARG:HA	1:G:93:PHE:N	2.31	0.46
1:H:99:GLN:HB3	1:H:100:GLY:HA3	1.98	0.46
1:A:226:PRO:HG2	1:A:229:LEU:HD12	1.98	0.46
1:C:204:GLY:HA2	1:C:217:GLY:O	2.16	0.46
1:F:91:ARG:HA	1:F:92:TRP:C	2.41	0.46
1:D:104:LEU:O	1:D:108:ARG:HG3	2.16	0.46
1:C:65:PRO:HB3	1:G:68:ALA:HA	1.97	0.46
1:C:228:MET:HE3	1:C:229:LEU:HG	1.98	0.46
1:E:159:PHE:HA	1:E:160:GLY:HA2	1.43	0.46
1:I:194:LYS:HG3	1:I:234:ALA:HB2	1.98	0.46
1:H:249:ARG:HB3	1:H:250:GLY:C	2.40	0.45
1:A:97:GLU:HG3	1:I:179:VAL:HG21	1.97	0.45
1:I:91:ARG:HA	1:I:93:PHE:N	2.32	0.45
1:D:72:SER:HB3	1:F:63:PHE:HB2	1.97	0.45
1:B:52:SER:HB2	1:B:134:ALA:HB3	1.98	0.45
1:E:107:GLU:HA	1:E:110:ILE:HD12	1.98	0.45
1:G:186:ILE:CG1	1:I:97:GLU:HG2	2.46	0.45
1:D:226:PRO:HB2	1:D:229:LEU:HB2	1.98	0.45
1:B:91:ARG:HA	1:B:92:TRP:C	2.41	0.45
1:F:82:MET:HE1	1:F:228:MET:O	2.16	0.45
1:D:60:THR:OG1	1:D:145:TYR:N	2.48	0.45
1:B:226:PRO:O	1:B:229:LEU:N	2.49	0.45
1:C:83:LEU:HD11	1:C:138:VAL:HG11	1.98	0.45
1:E:50:PHE:HD1	1:E:94:ILE:HB	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:96:LEU:HA	1:F:96:LEU:HD22	1.65	0.45
1:I:148:ASN:HB3	1:I:151:SER:HB3	1.99	0.45
1:I:208:PHE:HD1	1:I:208:PHE:HA	1.67	0.45
1:G:101:LEU:HD23	1:G:101:LEU:O	2.17	0.45
1:I:167:TYR:HA	1:I:198:SER:O	2.17	0.45
1:I:232:MET:O	1:I:236:GLU:N	2.49	0.45
1:A:46:THR:CB	1:A:47:GLY:HA3	2.46	0.45
1:E:51:VAL:HG11	1:E:87:LEU:HD13	1.99	0.45
1:E:53:VAL:HG22	1:E:80:THR:HG22	1.98	0.45
1:E:91:ARG:HA	1:E:92:TRP:C	2.42	0.45
1:D:76:PRO:HG2	1:D:228:MET:HA	1.98	0.45
1:A:159:PHE:HA	1:A:160:GLY:HA2	1.56	0.45
1:B:225:GLU:HA	1:B:226:PRO:HD3	1.78	0.45
1:F:94:ILE:O	1:F:96:LEU:HD23	2.17	0.45
1:I:177:ARG:HB3	1:I:189:SER:HB3	1.99	0.45
1:D:228:MET:HB3	1:D:228:MET:HE2	1.84	0.44
1:A:225:GLU:HA	1:A:226:PRO:HD3	1.64	0.44
1:H:91:ARG:HA	1:H:92:TRP:C	2.41	0.44
1:B:59:GLU:OE1	1:E:78:SER:HA	2.18	0.44
1:B:88:LYS:HD2	1:B:88:LYS:HA	1.85	0.44
1:F:107:GLU:OE1	1:H:98:ARG:NH1	2.51	0.44
1:H:97:GLU:HB3	1:H:98:ARG:H	1.48	0.44
1:D:157:ARG:HA	1:D:162:GLY:HA2	1.99	0.44
1:A:236:GLU:O	1:A:240:ILE:HG13	2.18	0.44
1:B:172:ILE:O	1:B:193:SER:HA	2.18	0.44
1:C:184:GLY:HA3	1:G:131:LEU:HD11	1.99	0.44
1:E:172:ILE:HG13	1:E:196:ILE:HD11	1.99	0.44
1:D:72:SER:HB3	1:F:63:PHE:N	2.33	0.44
1:H:64:LYS:HG2	1:H:74:ALA:HA	2.00	0.44
1:C:147:SER:HA	1:C:149:VAL:HG23	1.99	0.44
1:E:208:PHE:HD1	1:E:208:PHE:HA	1.69	0.44
1:I:170:ASP:O	1:I:195:THR:HA	2.17	0.44
1:A:246:GLY:HA3	1:A:252:TRP:CZ3	2.52	0.44
1:C:142:ILE:HD11	1:C:231:LEU:HD11	1.99	0.44
1:F:109:LYS:HA	1:F:112:ARG:NH1	2.33	0.44
1:D:82:MET:HE1	1:D:228:MET:O	2.18	0.44
1:E:137:MET:HB3	1:E:179:VAL:HG13	2.00	0.44
1:F:196:ILE:HG12	1:F:230:CYS:SG	2.57	0.44
1:G:66:TYR:CG	1:G:67:PRO:HA	2.53	0.44
1:I:91:ARG:HA	1:I:92:TRP:C	2.43	0.44
1:A:76:PRO:HG2	1:A:228:MET:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:TYR:HD1	1:B:172:ILE:HG12	1.82	0.43
1:G:104:LEU:O	1:G:108:ARG:HG3	2.18	0.43
1:G:159:PHE:HA	1:G:160:GLY:HA2	1.50	0.43
1:G:178:VAL:HG23	1:G:242:LEU:HD13	1.99	0.43
1:C:45:PRO:HG3	1:C:92:TRP:HZ2	1.83	0.43
1:C:133:ALA:CB	1:G:111:ILE:HG12	2.48	0.43
1:E:250:GLY:O	1:E:252:TRP:CD1	2.71	0.43
1:G:58:ASP:OD1	1:G:60:THR:HG22	2.18	0.43
1:A:98:ARG:NH2	1:B:110:ILE:HG21	2.34	0.43
1:E:88:LYS:HD2	1:E:88:LYS:HA	1.69	0.43
1:E:194:LYS:HE3	1:E:234:ALA:HA	2.00	0.43
1:F:56:ILE:CG2	1:F:80:THR:HG23	2.48	0.43
1:F:106:ASN:HA	1:F:109:LYS:NZ	2.33	0.43
1:G:137:MET:HE3	1:G:181:VAL:HG22	2.00	0.43
1:G:157:ARG:HA	1:G:162:GLY:HA2	1.99	0.43
1:E:60:THR:HG23	1:E:62:GLN:N	2.24	0.43
1:D:157:ARG:HD3	1:C:216:GLU:OE1	2.19	0.43
1:E:63:PHE:HB2	1:H:72:SER:HB3	2.00	0.43
1:E:105:LEU:HD23	1:E:105:LEU:HA	1.76	0.43
1:E:196:ILE:HD13	1:E:227:VAL:HG22	2.00	0.43
1:F:97:GLU:HG2	1:H:186:ILE:CG1	2.49	0.43
1:H:157:ARG:HA	1:H:162:GLY:HA2	2.01	0.43
1:F:68:ALA:HA	1:H:65:PRO:HB3	2.01	0.43
1:F:170:ASP:O	1:F:195:THR:HA	2.18	0.43
1:D:96:LEU:HD12	1:D:98:ARG:CZ	2.49	0.43
1:B:151:SER:HB2	1:B:168:GLN:HA	2.01	0.43
1:G:105:LEU:HA	1:G:105:LEU:HD23	1.76	0.43
1:G:175:ASN:HD21	1:I:85:THR:HG21	1.84	0.43
1:I:157:ARG:HA	1:I:162:GLY:HA2	1.99	0.43
1:B:60:THR:O	1:B:62:GLN:NE2	2.51	0.43
1:C:196:ILE:HD13	1:C:227:VAL:HA	2.01	0.43
1:C:244:ASN:HA	1:C:247:ILE:HG13	2.00	0.43
1:E:49:ILE:HD13	1:E:252:TRP:CE3	2.54	0.43
1:H:105:LEU:HD23	1:H:105:LEU:HA	1.77	0.43
1:A:176:LEU:HD12	1:A:176:LEU:HA	1.77	0.42
1:E:50:PHE:CD1	1:E:94:ILE:HB	2.54	0.42
1:F:245:ASP:OD1	1:F:245:ASP:N	2.52	0.42
1:I:231:LEU:O	1:I:235:ILE:N	2.43	0.42
1:B:99:GLN:HB3	1:B:100:GLY:HA3	2.01	0.42
1:C:53:VAL:HG22	1:C:80:THR:HG22	2.00	0.42
1:G:51:VAL:HG11	1:G:87:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:SER:OG	1:C:85:THR:HG22	2.19	0.42
1:E:178:VAL:HG23	1:E:242:LEU:HD13	2.00	0.42
1:E:249:ARG:HB3	1:E:250:GLY:C	2.44	0.42
1:B:159:PHE:HA	1:B:160:GLY:HA2	1.48	0.42
1:C:147:SER:HB3	1:C:170:ASP:CG	2.43	0.42
1:C:226:PRO:O	1:C:229:LEU:N	2.44	0.42
1:F:148:ASN:HB3	1:F:151:SER:HB3	2.01	0.42
1:G:177:ARG:HG2	1:G:189:SER:CB	2.49	0.42
1:H:169:LEU:HA	1:H:196:ILE:O	2.19	0.42
1:D:69:SER:O	1:D:72:SER:OG	2.37	0.42
1:A:97:GLU:HB3	1:A:98:ARG:H	1.53	0.42
1:A:157:ARG:HA	1:A:162:GLY:HA2	2.01	0.42
1:E:42:LEU:HA	1:E:43:PRO:HD3	1.83	0.42
1:E:250:GLY:C	1:E:252:TRP:H	2.27	0.42
1:F:130:SER:OG	1:F:131:LEU:N	2.53	0.42
1:A:75:VAL:HA	1:A:76:PRO:HD3	1.97	0.42
1:C:179:VAL:HB	1:C:186:ILE:HG12	2.01	0.42
1:F:140:GLY:HA3	1:F:175:ASN:O	2.19	0.42
1:H:246:GLY:O	1:H:250:GLY:HA2	2.19	0.42
1:A:52:SER:HB2	1:A:98:ARG:HH11	1.85	0.42
1:A:186:ILE:HG12	1:B:97:GLU:HG2	2.01	0.42
1:C:172:ILE:O	1:C:193:SER:HA	2.20	0.42
1:E:106:ASN:O	1:E:110:ILE:HG13	2.20	0.42
1:E:172:ILE:O	1:E:193:SER:HA	2.19	0.42
1:F:91:ARG:HA	1:F:93:PHE:N	2.35	0.42
1:G:52:SER:OG	1:G:98:ARG:NH1	2.46	0.42
1:I:225:GLU:HA	1:I:226:PRO:HD3	1.58	0.42
1:D:73:THR:HG21	1:D:77:GLN:NE2	2.34	0.42
1:D:157:ARG:HH22	1:D:206:PHE:HB2	1.85	0.42
1:A:138:VAL:HA	1:A:177:ARG:O	2.20	0.42
1:H:58:ASP:HB3	1:H:77:GLN:NE2	2.35	0.42
1:I:56:ILE:HG13	1:I:141:SER:HA	2.02	0.42
1:B:157:ARG:HA	1:B:162:GLY:HA2	2.02	0.42
1:B:175:ASN:HA	1:B:190:VAL:O	2.19	0.42
1:G:105:LEU:O	1:G:109:LYS:HG3	2.20	0.42
1:A:82:MET:HA	1:A:232:MET:HE1	2.02	0.42
1:C:60:THR:HG23	1:C:62:GLN:H	1.85	0.42
1:E:194:LYS:HG2	1:E:234:ALA:HB2	2.02	0.42
1:F:51:VAL:HG22	1:F:53:VAL:HG12	2.02	0.42
1:F:76:PRO:HG2	1:F:228:MET:HA	2.01	0.42
1:A:52:SER:O	1:A:137:MET:HG3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:46:THR:OG1	1:E:252:TRP:O	2.27	0.41
1:F:248:ASP:OD1	1:F:248:ASP:N	2.52	0.41
1:H:105:LEU:O	1:H:109:LYS:HG3	2.20	0.41
1:H:232:MET:O	1:H:235:ILE:HG22	2.19	0.41
1:I:204:GLY:HA2	1:I:217:GLY:O	2.20	0.41
1:D:96:LEU:HA	1:D:96:LEU:HD22	1.67	0.41
1:B:137:MET:HE3	1:B:137:MET:HB2	1.76	0.41
1:C:60:THR:HG23	1:C:62:GLN:N	2.34	0.41
1:C:159:PHE:HA	1:C:160:GLY:HA2	1.54	0.41
1:E:157:ARG:HA	1:E:162:GLY:HA2	2.02	0.41
1:A:171:GLN:HG2	1:A:195:THR:HG22	2.02	0.41
1:A:172:ILE:CG1	1:A:196:ILE:HD11	2.49	0.41
1:C:107:GLU:O	1:C:111:ILE:HG13	2.20	0.41
1:E:83:LEU:O	1:E:87:LEU:HG	2.20	0.41
1:I:58:ASP:OD1	1:I:60:THR:HG22	2.21	0.41
1:A:244:ASN:O	1:A:247:ILE:HB	2.21	0.41
1:E:179:VAL:HG21	1:H:97:GLU:HG3	2.02	0.41
1:F:157:ARG:HH22	1:F:206:PHE:HD2	1.67	0.41
1:D:178:VAL:HG23	1:D:242:LEU:HD22	2.03	0.41
1:E:174:VAL:HG12	1:E:176:LEU:HD13	2.02	0.41
1:H:178:VAL:HG12	1:H:187:LEU:HB2	2.03	0.41
1:H:215:LEU:HD23	1:H:216:GLU:N	2.36	0.41
1:D:97:GLU:HB3	1:D:98:ARG:H	1.56	0.41
1:A:176:LEU:HB3	1:A:242:LEU:HD11	2.02	0.41
1:B:94:ILE:HD13	1:B:94:ILE:HA	1.89	0.41
1:B:178:VAL:HG23	1:B:242:LEU:HD13	2.02	0.41
1:H:98:ARG:HG3	1:H:101:LEU:HD12	2.03	0.41
1:I:243:ILE:O	1:I:247:ILE:HG13	2.20	0.41
1:I:249:ARG:N	1:I:250:GLY:HA2	2.36	0.41
1:D:175:ASN:HA	1:D:190:VAL:O	2.20	0.41
1:A:154:VAL:HG12	1:B:219:VAL:HG12	2.01	0.41
1:I:172:ILE:O	1:I:193:SER:HA	2.21	0.41
1:D:132:THR:HG23	1:F:183:THR:HB	2.02	0.41
1:A:77:GLN:HB2	1:I:59:GLU:O	2.21	0.41
1:A:246:GLY:HA3	1:A:252:TRP:CH2	2.56	0.41
1:C:180:ASN:HB2	1:C:187:LEU:HD11	2.02	0.41
1:C:230:CYS:O	1:C:234:ALA:N	2.40	0.41
1:C:249:ARG:HB3	1:C:250:GLY:O	2.20	0.41
1:E:98:ARG:HD2	1:E:98:ARG:N	2.36	0.41
1:G:88:LYS:HD3	1:G:95:PRO:HD2	2.03	0.41
1:I:50:PHE:HD1	1:I:50:PHE:HA	1.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:ILE:HG12	1:F:133:ALA:CB	2.50	0.41
1:A:104:LEU:HA	1:I:137:MET:HE1	2.02	0.41
1:E:58:ASP:OD1	1:E:60:THR:HG22	2.20	0.41
1:E:184:GLY:HA3	1:H:131:LEU:HD11	2.01	0.41
1:E:186:ILE:HD12	1:H:95:PRO:HB2	2.02	0.41
1:F:110:ILE:HG21	1:H:98:ARG:HH22	1.85	0.41
1:F:147:SER:HA	1:F:149:VAL:HG23	2.02	0.41
1:F:199:TYR:CE1	1:F:223:SER:HB3	2.56	0.41
1:G:107:GLU:O	1:G:111:ILE:HG13	2.21	0.41
1:G:186:ILE:HG12	1:I:97:GLU:HG2	2.03	0.41
1:H:208:PHE:HD1	1:H:208:PHE:HA	1.68	0.41
1:I:169:LEU:HA	1:I:196:ILE:O	2.20	0.41
1:D:51:VAL:HG11	1:D:87:LEU:HD13	2.01	0.41
1:A:245:ASP:O	1:A:249:ARG:HB2	2.21	0.41
1:C:252:TRP:CD1	1:C:252:TRP:N	2.89	0.41
1:I:93:PHE:HD1	1:I:93:PHE:HA	1.80	0.41
1:A:78:SER:HB2	1:A:82:MET:HG3	2.01	0.40
1:C:138:VAL:HA	1:C:177:ARG:O	2.21	0.40
1:G:98:ARG:HA	1:G:101:LEU:HB2	2.02	0.40
1:G:184:GLY:HA3	1:I:131:LEU:HD11	2.03	0.40
1:H:82:MET:HE1	1:H:228:MET:O	2.22	0.40
1:H:180:ASN:HB2	1:H:187:LEU:HD21	2.03	0.40
1:A:146:GLU:OE1	1:B:228:MET:HB3	2.21	0.40
1:C:96:LEU:O	1:C:98:ARG:HD2	2.21	0.40
1:E:143:ILE:CG2	1:H:82:MET:HE3	2.52	0.40
1:F:75:VAL:HA	1:F:76:PRO:HD3	1.96	0.40
1:F:82:MET:HE2	1:F:232:MET:HE2	2.04	0.40
1:G:226:PRO:HG2	1:G:229:LEU:HD12	2.02	0.40
1:H:60:THR:HG23	1:H:62:GLN:N	2.34	0.40
1:A:172:ILE:CD1	1:A:196:ILE:HD11	2.51	0.40
1:B:147:SER:HB3	1:B:170:ASP:CG	2.46	0.40
1:F:149:VAL:HG11	1:F:171:GLN:HE21	1.86	0.40
1:G:53:VAL:HG21	1:G:83:LEU:HD12	2.03	0.40
1:D:85:THR:HG22	1:F:189:SER:OG	2.21	0.40
1:D:137:MET:HE3	1:D:137:MET:HB2	1.67	0.40
1:A:235:ILE:O	1:A:239:VAL:HG23	2.21	0.40
1:G:180:ASN:OD1	1:G:183:THR:N	2.44	0.40
1:H:137:MET:HE3	1:H:137:MET:HB2	1.82	0.40
1:I:78:SER:O	1:I:81:ALA:HB3	2.21	0.40
1:A:190:VAL:HG12	1:A:192:THR:HG23	2.03	0.40
1:A:242:LEU:HA	1:A:242:LEU:HD23	1.84	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	190/277 (69%)	177 (93%)	12 (6%)	1 (0%)	24	57
1	B	184/277 (66%)	175 (95%)	8 (4%)	1 (0%)	24	57
1	C	192/277 (69%)	176 (92%)	15 (8%)	1 (0%)	24	57
1	D	183/277 (66%)	173 (94%)	9 (5%)	1 (0%)	24	57
1	E	192/277 (69%)	174 (91%)	17 (9%)	1 (0%)	24	57
1	F	183/277 (66%)	174 (95%)	8 (4%)	1 (0%)	24	57
1	G	184/277 (66%)	174 (95%)	9 (5%)	1 (0%)	24	57
1	H	185/277 (67%)	174 (94%)	10 (5%)	1 (0%)	24	57
1	I	184/277 (66%)	176 (96%)	7 (4%)	1 (0%)	24	57
All	All	1677/2493 (67%)	1573 (94%)	95 (6%)	9 (0%)	24	57

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	149	VAL
1	A	149	VAL
1	B	149	VAL
1	C	149	VAL
1	E	149	VAL
1	F	149	VAL
1	G	149	VAL
1	H	149	VAL
1	I	149	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	157/236 (66%)	132 (84%)	25 (16%)	2	12
1	B	153/236 (65%)	126 (82%)	27 (18%)	2	9
1	C	160/236 (68%)	135 (84%)	25 (16%)	2	12
1	D	153/236 (65%)	131 (86%)	22 (14%)	3	14
1	E	160/236 (68%)	128 (80%)	32 (20%)	1	6
1	F	153/236 (65%)	126 (82%)	27 (18%)	2	9
1	G	155/236 (66%)	130 (84%)	25 (16%)	2	11
1	H	154/236 (65%)	129 (84%)	25 (16%)	2	11
1	I	153/236 (65%)	125 (82%)	28 (18%)	2	8
All	All	1398/2124 (66%)	1162 (83%)	236 (17%)	2	10

All (236) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	49	ILE
1	D	51	VAL
1	D	53	VAL
1	D	62	GLN
1	D	75	VAL
1	D	78	SER
1	D	80	THR
1	D	89	ASP
1	D	92	TRP
1	D	96	LEU
1	D	97	GLU
1	D	105	LEU
1	D	139	GLU
1	D	141	SER
1	D	146	GLU
1	D	164	ASP
1	D	176	LEU
1	D	179	VAL

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Mol	Chain	Res	Type
1	D	193	SER
1	D	198	SER
1	D	208	PHE
1	D	216	GLU
1	A	49	ILE
1	A	51	VAL
1	A	53	VAL
1	A	56	ILE
1	A	62	GLN
1	A	69	SER
1	A	75	VAL
1	A	78	SER
1	A	80	THR
1	A	83	LEU
1	A	96	LEU
1	A	97	GLU
1	A	101	LEU
1	A	105	LEU
1	A	132	THR
1	A	139	GLU
1	A	146	GLU
1	A	165	THR
1	A	176	LEU
1	A	179	VAL
1	A	193	SER
1	A	198	SER
1	A	208	PHE
1	A	248	ASP
1	A	251	LEU
1	B	49	ILE
1	B	53	VAL
1	B	56	ILE
1	B	62	GLN
1	B	69	SER
1	B	75	VAL
1	B	77	GLN
1	B	78	SER
1	B	80	THR
1	B	93	PHE
1	B	96	LEU
1	B	105	LEU
1	B	131	LEU

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Mol	Chain	Res	Type
1	B	139	GLU
1	B	141	SER
1	B	147	SER
1	B	165	THR
1	B	176	LEU
1	B	177	ARG
1	B	179	VAL
1	B	186	ILE
1	B	193	SER
1	B	198	SER
1	B	208	PHE
1	B	228	MET
1	B	244	ASN
1	B	251	LEU
1	C	41	HIS
1	C	42	LEU
1	C	49	ILE
1	C	56	ILE
1	C	62	GLN
1	C	64	LYS
1	C	69	SER
1	C	78	SER
1	C	80	THR
1	C	96	LEU
1	C	97	GLU
1	C	105	LEU
1	C	139	GLU
1	C	141	SER
1	C	151	SER
1	C	169	LEU
1	C	176	LEU
1	C	177	ARG
1	C	179	VAL
1	C	193	SER
1	C	198	SER
1	C	208	PHE
1	C	248	ASP
1	C	251	LEU
1	C	252	TRP
1	E	42	LEU
1	E	49	ILE
1	E	53	VAL

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Mol	Chain	Res	Type
1	E	56	ILE
1	E	57	GLN
1	E	62	GLN
1	E	69	SER
1	E	78	SER
1	E	80	THR
1	E	83	LEU
1	E	96	LEU
1	E	97	GLU
1	E	105	LEU
1	E	111	ILE
1	E	131	LEU
1	E	136	ILE
1	E	139	GLU
1	E	143	ILE
1	E	146	GLU
1	E	151	SER
1	E	165	THR
1	E	172	ILE
1	E	176	LEU
1	E	179	VAL
1	E	190	VAL
1	E	208	PHE
1	E	216	GLU
1	E	228	MET
1	E	230	CYS
1	E	237	THR
1	E	248	ASP
1	E	251	LEU
1	F	49	ILE
1	F	50	PHE
1	F	51	VAL
1	F	53	VAL
1	F	56	ILE
1	F	62	GLN
1	F	64	LYS
1	F	75	VAL
1	F	77	GLN
1	F	78	SER
1	F	80	THR
1	F	83	LEU
1	F	96	LEU

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Mol	Chain	Res	Type
1	F	97	GLU
1	F	105	LEU
1	F	111	ILE
1	F	130	SER
1	F	136	ILE
1	F	139	GLU
1	F	146	GLU
1	F	151	SER
1	F	165	THR
1	F	176	LEU
1	F	179	VAL
1	F	193	SER
1	F	208	PHE
1	F	248	ASP
1	G	49	ILE
1	G	50	PHE
1	G	56	ILE
1	G	62	GLN
1	G	77	GLN
1	G	78	SER
1	G	83	LEU
1	G	97	GLU
1	G	130	SER
1	G	131	LEU
1	G	136	ILE
1	G	139	GLU
1	G	142	ILE
1	G	146	GLU
1	G	151	SER
1	G	165	THR
1	G	176	LEU
1	G	179	VAL
1	G	198	SER
1	G	208	PHE
1	G	214	LEU
1	G	228	MET
1	G	230	CYS
1	G	231	LEU
1	G	248	ASP
1	H	49	ILE
1	H	51	VAL
1	H	53	VAL

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Mol	Chain	Res	Type
1	H	56	ILE
1	H	62	GLN
1	H	77	GLN
1	H	80	THR
1	H	83	LEU
1	H	93	PHE
1	H	97	GLU
1	H	101	LEU
1	H	130	SER
1	H	131	LEU
1	H	139	GLU
1	H	146	GLU
1	H	151	SER
1	H	165	THR
1	H	176	LEU
1	H	179	VAL
1	H	200	GLU
1	H	208	PHE
1	H	230	CYS
1	H	237	THR
1	H	248	ASP
1	H	251	LEU
1	I	49	ILE
1	I	50	PHE
1	I	51	VAL
1	I	53	VAL
1	I	56	ILE
1	I	62	GLN
1	I	75	VAL
1	I	78	SER
1	I	80	THR
1	I	93	PHE
1	I	96	LEU
1	I	105	LEU
1	I	130	SER
1	I	132	THR
1	I	136	ILE
1	I	138	VAL
1	I	139	GLU
1	I	146	GLU
1	I	151	SER
1	I	165	THR

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Mol	Chain	Res	Type
1	I	176	LEU
1	I	177	ARG
1	I	179	VAL
1	I	186	ILE
1	I	208	PHE
1	I	216	GLU
1	I	248	ASP
1	I	251	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	77	GLN
1	D	102	GLN
1	D	224	ASN
1	B	175	ASN
1	B	244	ASN
1	C	175	ASN
1	C	244	ASN
1	E	57	GLN
1	E	224	ASN
1	F	99	GLN
1	F	102	GLN
1	F	171	GLN
1	H	77	GLN
1	I	224	ASN

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

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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

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	196/277 (70%)	0.58	11 (5%)	30	16	43, 79, 133, 179	0
1	B	190/277 (68%)	0.59	15 (7%)	18	10	42, 82, 145, 179	0
1	C	198/277 (71%)	0.53	12 (6%)	27	15	31, 73, 143, 173	0
1	D	189/277 (68%)	0.52	9 (4%)	35	19	42, 77, 129, 161	0
1	E	198/277 (71%)	0.60	15 (7%)	20	11	31, 78, 142, 161	0
1	F	189/277 (68%)	0.52	18 (9%)	14	7	29, 77, 140, 166	0
1	G	190/277 (68%)	0.65	12 (6%)	26	14	40, 82, 146, 166	0
1	H	191/277 (68%)	0.60	15 (7%)	18	10	38, 80, 144, 164	0
1	I	190/277 (68%)	0.67	15 (7%)	18	10	42, 77, 150, 181	0
All	All	1731/2493 (69%)	0.58	122 (7%)	22	12	29, 78, 144, 181	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	49	ILE	5.0
1	I	247	ILE	3.9
1	A	148	ASN	3.9
1	A	78	SER	3.8
1	F	209	ILE	3.7
1	B	213	ARG	3.7
1	D	247	ILE	3.6
1	I	106	ASN	3.6
1	C	70	ASN	3.5
1	E	171	GLN	3.5
1	A	169	LEU	3.5
1	B	158	TYR	3.4
1	H	135	ASN	3.4
1	D	158	TYR	3.3
1	F	240	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	158	TYR	3.3
1	G	102	GLN	3.2
1	C	171	GLN	3.2
1	G	92	TRP	3.2
1	C	42	LEU	3.1
1	A	168	GLN	3.1
1	F	78	SER	3.1
1	E	78	SER	3.1
1	B	98	ARG	3.1
1	B	97	GLU	3.0
1	I	147	SER	3.0
1	I	115	GLN	3.0
1	G	196	ILE	2.9
1	B	102	GLN	2.9
1	B	74	ALA	2.9
1	E	151	SER	2.9
1	D	78	SER	2.8
1	C	44	ALA	2.8
1	C	148	ASN	2.8
1	H	159	PHE	2.8
1	G	49	ILE	2.8
1	F	102	GLN	2.7
1	H	213	ARG	2.7
1	F	76	PRO	2.7
1	E	247	ILE	2.7
1	C	52	SER	2.7
1	E	193	SER	2.7
1	H	153	GLY	2.7
1	D	199	TYR	2.7
1	B	214	LEU	2.7
1	F	214	LEU	2.7
1	I	158	TYR	2.7
1	F	148	ASN	2.7
1	H	143	ILE	2.6
1	C	206	PHE	2.6
1	I	102	GLN	2.6
1	F	55	ASN	2.6
1	E	150	LYS	2.6
1	F	247	ILE	2.6
1	B	54	TYR	2.5
1	C	158	TYR	2.5
1	B	101	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	252	TRP	2.5
1	H	58	ASP	2.5
1	B	89	ASP	2.5
1	B	145	TYR	2.5
1	E	64	LYS	2.5
1	F	158	TYR	2.5
1	H	74	ALA	2.5
1	E	236	GLU	2.5
1	G	159	PHE	2.5
1	B	73	THR	2.5
1	I	209	ILE	2.4
1	A	158	TYR	2.4
1	F	92	TRP	2.4
1	D	213	ARG	2.4
1	H	225	GLU	2.4
1	E	132	THR	2.4
1	D	229	LEU	2.3
1	D	97	GLU	2.3
1	F	213	ARG	2.3
1	I	207	ARG	2.3
1	C	247	ILE	2.3
1	G	110	ILE	2.3
1	H	163	ALA	2.3
1	F	80	THR	2.3
1	A	83	LEU	2.3
1	G	251	LEU	2.3
1	I	159	PHE	2.3
1	I	111	ILE	2.2
1	I	113	ALA	2.2
1	F	132	THR	2.2
1	C	130	SER	2.2
1	H	51	VAL	2.2
1	A	49	ILE	2.2
1	A	213	ARG	2.2
1	E	213	ARG	2.2
1	G	158	TYR	2.2
1	F	129	GLN	2.2
1	D	197	LEU	2.2
1	A	59	GLU	2.1
1	B	159	PHE	2.1
1	G	106	ASN	2.1
1	H	70	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	85	THR	2.1
1	C	213	ARG	2.1
1	H	178	VAL	2.1
1	A	170	ASP	2.1
1	B	56	ILE	2.1
1	H	49	ILE	2.1
1	H	145	TYR	2.1
1	A	171	GLN	2.1
1	H	218	GLU	2.1
1	I	48	LYS	2.1
1	E	111	ILE	2.1
1	F	250	GLY	2.1
1	E	159	PHE	2.1
1	C	235	ILE	2.0
1	I	228	MET	2.0
1	E	44	ALA	2.0
1	I	145	TYR	2.0
1	F	168	GLN	2.0
1	G	225	GLU	2.0
1	G	213	ARG	2.0
1	F	217	GLY	2.0
1	B	251	LEU	2.0
1	E	169	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 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HG	B	501	1/1	0.92	0.08	147,147,147,147	1
2	HG	A	501	1/1	0.93	0.07	121,121,121,121	1
2	HG	D	501	1/1	0.93	0.09	115,115,115,115	1
2	HG	I	501	1/1	0.94	0.09	181,181,181,181	0
2	HG	H	501	1/1	0.96	0.07	166,166,166,166	1
2	HG	G	501	1/1	0.97	0.07	161,161,161,161	0
2	HG	E	501	1/1	0.97	0.04	127,127,127,127	0
2	HG	F	501	1/1	0.97	0.09	130,130,130,130	1
2	HG	C	501	1/1	0.98	0.05	137,137,137,137	0

6.5 Other polymers [i](#)

There are no such residues in this entry.