



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 04:18 PM UTC

PDB ID : 8JEN / pdb_00008jen
Title : Crystal structure of TIGIT in complexed with Ociperlimab, crystal form II
Authors : Sun, J.; Zhang, X.X.; Song, J.
Deposited on : 2023-05-16
Resolution : 2.71 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

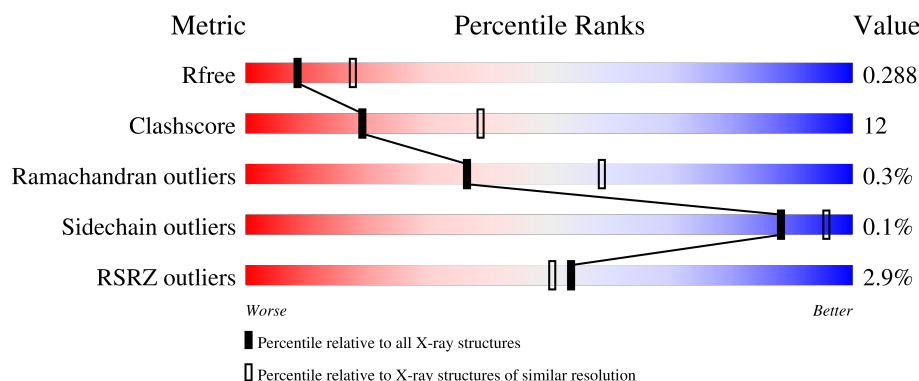
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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	222	70%27%.
1	C	222	4% 76%22%.
1	E	222	% 73%24%.
1	G	222	3% 69%27%..
2	B	214	2% 76%23%

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Mol	Chain	Length	Quality of chain
2	D	214	3% 70% 29%
2	F	214	2% 75% 24%
2	H	214	2% 77% 23%
3	I	115	3% 74% 18% 8%
3	J	115	2% 74% 18% 8%
3	M	115	10% 71% 19% 8%
3	P	115	8% 64% 25% 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16736 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 antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1640	1040	270	322	8			
1	C	217	Total	C	N	O	S	0	0	0
			1640	1040	270	322	8			
1	E	217	Total	C	N	O	S	0	0	0
			1640	1040	270	322	8			
1	G	217	Total	C	N	O	S	0	0	0
			1640	1040	270	322	8			

- Molecule 2 is a protein called antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1638	1027	275	330	6			
2	D	214	Total	C	N	O	S	0	0	0
			1638	1027	275	330	6			
2	F	214	Total	C	N	O	S	0	0	0
			1638	1027	275	330	6			
2	H	214	Total	C	N	O	S	0	0	0
			1638	1027	275	330	6			

- Molecule 3 is a protein called T-cell immunoreceptor with Ig and ITIM domains.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	106	Total	C	N	O	S	0	0	0
			811	511	133	163	4			
3	J	106	Total	C	N	O	S	0	0	0
			811	511	133	163	4			
3	M	106	Total	C	N	O	S	0	0	0
			811	511	133	163	4			
3	P	104	Total	C	N	O	S	0	0	0
			796	502	131	160	3			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	129	LEU	-	expression tag	UNP Q495A1
I	130	GLU	-	expression tag	UNP Q495A1
I	131	HIS	-	expression tag	UNP Q495A1
I	132	HIS	-	expression tag	UNP Q495A1
I	133	HIS	-	expression tag	UNP Q495A1
I	134	HIS	-	expression tag	UNP Q495A1
I	135	HIS	-	expression tag	UNP Q495A1
I	136	HIS	-	expression tag	UNP Q495A1
J	129	LEU	-	expression tag	UNP Q495A1
J	130	GLU	-	expression tag	UNP Q495A1
J	131	HIS	-	expression tag	UNP Q495A1
J	132	HIS	-	expression tag	UNP Q495A1
J	133	HIS	-	expression tag	UNP Q495A1
J	134	HIS	-	expression tag	UNP Q495A1
J	135	HIS	-	expression tag	UNP Q495A1
J	136	HIS	-	expression tag	UNP Q495A1
M	129	LEU	-	expression tag	UNP Q495A1
M	130	GLU	-	expression tag	UNP Q495A1
M	131	HIS	-	expression tag	UNP Q495A1
M	132	HIS	-	expression tag	UNP Q495A1
M	133	HIS	-	expression tag	UNP Q495A1
M	134	HIS	-	expression tag	UNP Q495A1
M	135	HIS	-	expression tag	UNP Q495A1
M	136	HIS	-	expression tag	UNP Q495A1
P	129	LEU	-	expression tag	UNP Q495A1
P	130	GLU	-	expression tag	UNP Q495A1
P	131	HIS	-	expression tag	UNP Q495A1
P	132	HIS	-	expression tag	UNP Q495A1
P	133	HIS	-	expression tag	UNP Q495A1
P	134	HIS	-	expression tag	UNP Q495A1
P	135	HIS	-	expression tag	UNP Q495A1
P	136	HIS	-	expression tag	UNP Q495A1

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	35	Total O 35 35	0	0
4	B	48	Total O 48 48	0	0
4	C	31	Total O 31 31	0	0

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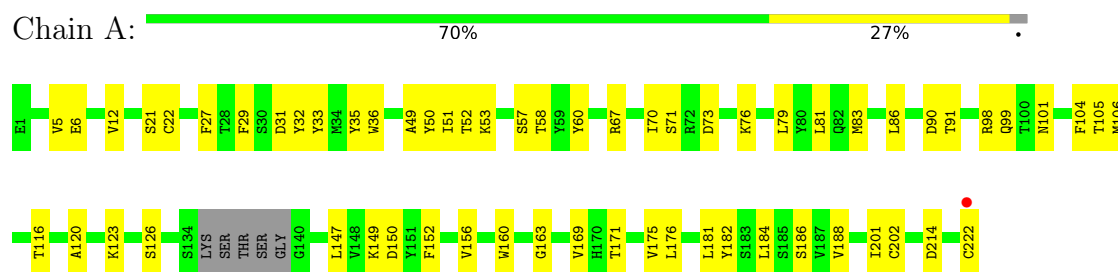
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	51	Total 51	O 51	0	0
4	E	41	Total 41	O 41	0	0
4	F	44	Total 44	O 44	0	0
4	I	24	Total 24	O 24	0	0
4	J	16	Total 16	O 16	0	0
4	M	17	Total 17	O 17	0	0
4	P	13	Total 13	O 13	0	0
4	G	33	Total 33	O 33	0	0
4	H	42	Total 42	O 42	0	0

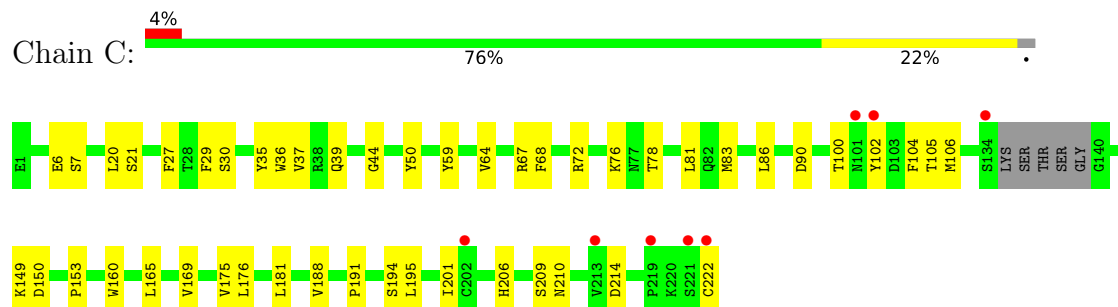
3 Residue-property plots [i](#)

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.

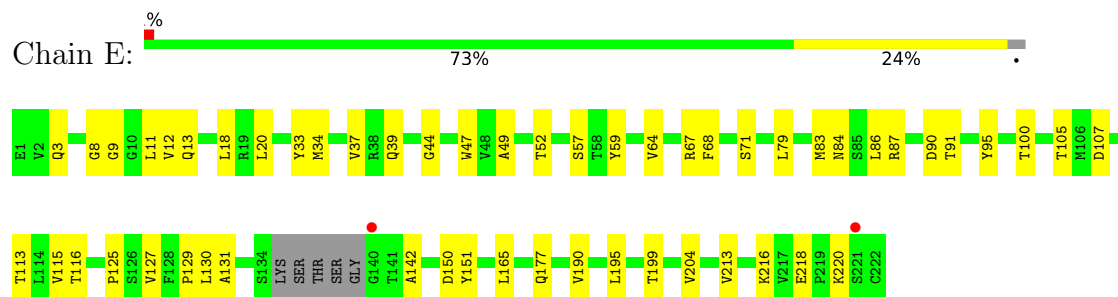
- Molecule 1: antibody heavy chain



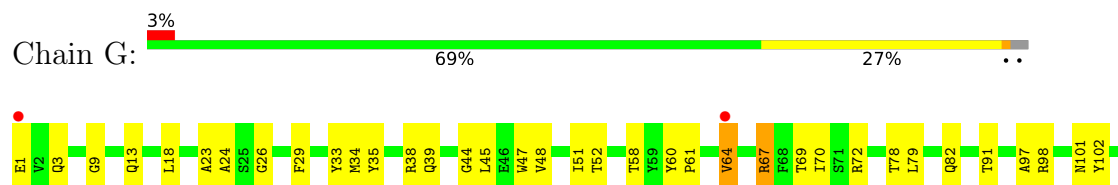
- Molecule 1: antibody heavy chain

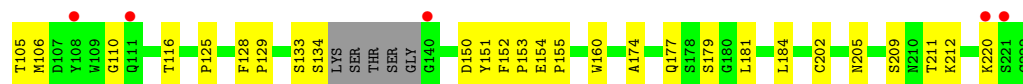


- Molecule 1: antibody heavy chain

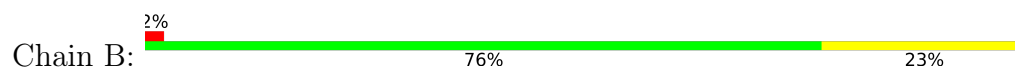


- Molecule 1: antibody heavy chain

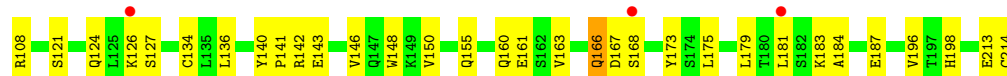
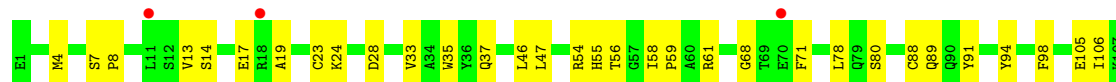
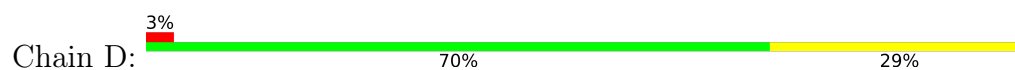




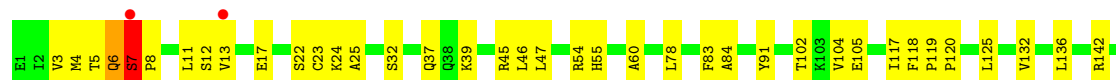
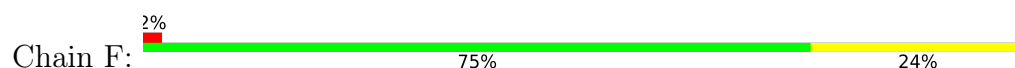
- Molecule 2: antibody light chain



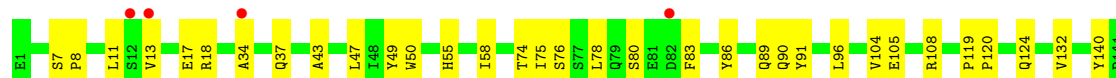
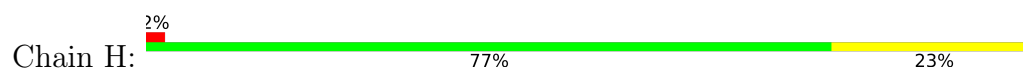
- Molecule 2: antibody light chain



- Molecule 2: antibody light chain



- Molecule 2: antibody light chain

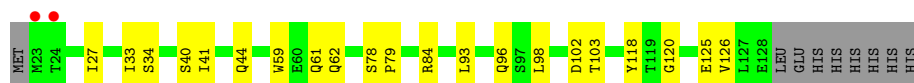
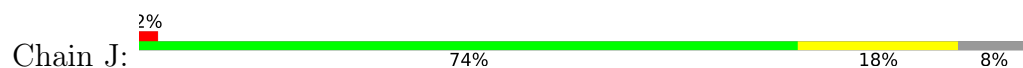


- Molecule 3: T-cell immunoreceptor with Ig and ITIM domains

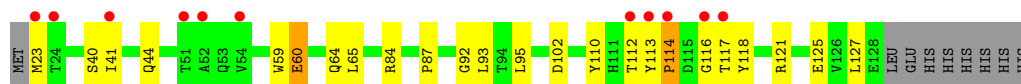
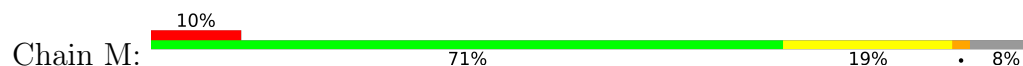




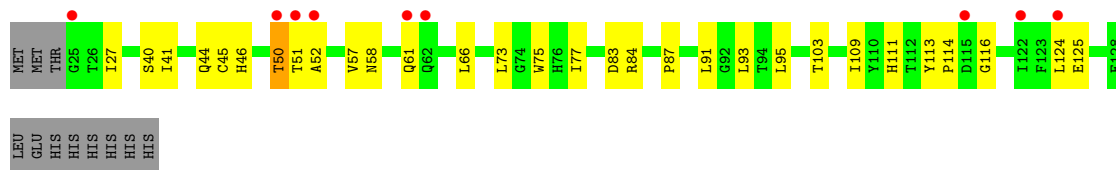
- Molecule 3: T-cell immunoreceptor with Ig and ITIM domains



- Molecule 3: T-cell immunoreceptor with Ig and ITIM domains



- Molecule 3: T-cell immunoreceptor with Ig and ITIM domains



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	100.32Å 79.35Å 173.69Å 90.00° 101.67° 90.00°	Depositor
Resolution (Å)	49.12 – 2.71 49.12 – 2.71	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.12-2.71) 99.8 (49.12-2.71)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 2.73Å)	Xtriage
Refinement program	PHENIX (1.17.1_3660: ???)	Depositor
R, R_{free}	0.218 , 0.289 0.219 , 0.288	Depositor DCC
R_{free} test set	3677 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	46.4	Xtriage
Anisotropy	0.714	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16736	wwPDB-VP
Average B, all atoms (Å ²)	47.0	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 48.03 % 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 9.1165e-05. 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

5.1 Standard geometry

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	0/1681	0.65	0/2290
1	C	0.39	0/1681	0.63	0/2290
1	E	0.40	0/1681	0.64	0/2290
1	G	0.40	0/1681	0.66	0/2290
2	B	0.41	0/1675	0.63	0/2276
2	D	0.39	0/1675	0.59	0/2276
2	F	0.38	0/1675	0.62	0/2276
2	H	0.38	0/1675	0.61	0/2276
3	I	0.42	0/828	0.67	0/1130
3	J	0.36	0/828	0.60	0/1130
3	M	0.41	0/828	0.69	0/1130
3	P	0.39	0/813	0.68	0/1110
All	All	0.39	0/16721	0.64	0/22764

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
2	B	0	1
2	D	0	1
2	F	0	2
3	M	0	1
3	P	0	2
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	213	GLU	Peptide
2	D	166	GLN	Peptide
2	F	6	GLN	Peptide
2	F	7	SER	Peptide
3	M	60	GLU	Peptide
3	P	113	TYR	Peptide
3	P	50	THR	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1640	0	1592	47	0
1	C	1640	0	1592	39	0
1	E	1640	0	1591	38	0
1	G	1640	0	1591	49	0
2	B	1638	0	1589	39	0
2	D	1638	0	1589	43	0
2	F	1638	0	1588	42	0
2	H	1638	0	1588	40	0
3	I	811	0	779	15	0
3	J	811	0	779	17	1
3	M	811	0	779	16	0
3	P	796	0	763	19	1
4	A	35	0	0	6	0
4	B	48	0	0	6	0
4	C	31	0	0	3	0
4	D	51	0	0	1	1
4	E	41	0	0	6	0
4	F	44	0	0	4	0
4	G	33	0	0	3	1
4	H	42	0	0	4	0
4	I	24	0	0	0	0
4	J	16	0	0	0	0
4	M	17	0	0	2	0
4	P	13	0	0	0	0
All	All	16736	0	15820	375	2

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 12.

All (375) 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:E:190:VAL:O	4:E:301:HOH:O	1.86	0.92
1:G:179:SER:HB3	1:G:181:LEU:HD12	1.56	0.87
2:F:155:GLN:HB3	2:F:158:ASN:HD21	1.40	0.86
1:G:101:ASN:ND2	4:G:301:HOH:O	2.09	0.85
3:I:25:GLY:HA2	3:I:49:SER:HB2	1.60	0.82
2:F:12:SER:OG	2:F:105:GLU:OE1	2.00	0.79
1:E:12:VAL:HG11	1:E:86:LEU:HD13	1.65	0.78
2:H:18:ARG:NH2	2:H:74:THR:HG21	1.99	0.76
2:H:182:SER:HB2	2:H:185:ASP:H	1.51	0.76
1:A:123:LYS:NZ	4:A:302:HOH:O	2.19	0.75
3:M:113:TYR:HB3	3:M:114:PRO:HD3	1.68	0.75
1:G:91:THR:HG23	1:G:116:THR:HA	1.71	0.72
2:B:47:LEU:HD23	2:B:58:ILE:HD12	1.72	0.72
1:C:35:TYR:CE2	1:C:106:MET:HG2	2.26	0.70
2:F:7:SER:HG	2:F:102:THR:HG1	1.39	0.69
3:I:112:THR:HB	3:I:116:GLY:O	1.93	0.69
2:H:161:GLU:HG2	2:H:175:LEU:HD21	1.75	0.68
2:H:11:LEU:HB3	2:H:104:VAL:HG13	1.74	0.68
3:M:60:GLU:HG2	3:M:65:LEU:HD13	1.75	0.68
2:H:153:ALA:O	2:H:155:GLN:NE2	2.26	0.68
2:F:155:GLN:HB3	2:F:158:ASN:ND2	2.08	0.67
2:B:124:GLN:O	2:B:127:SER:HB3	1.94	0.67
1:C:175:VAL:HG11	2:D:160:GLN:HB3	1.75	0.67
2:D:37:GLN:HB2	2:D:47:LEU:HD11	1.76	0.67
1:G:51:ILE:HG13	1:G:58:THR:HG22	1.76	0.67
1:A:147:LEU:HD21	1:A:149:LYS:HD2	1.75	0.67
2:H:13:VAL:HG12	2:H:17:GLU:HB3	1.76	0.67
2:H:214:CYS:O	4:H:301:HOH:O	2.13	0.66
3:J:33:ILE:HG21	3:J:41:ILE:HD12	1.78	0.65
1:E:67:ARG:NH1	1:E:90:ASP:OD2	2.29	0.65
1:A:222:CYS:HB3	2:B:214:CYS:SG	2.37	0.65
2:D:163:VAL:HG22	2:D:175:LEU:HD12	1.78	0.65
2:B:191:VAL:O	4:B:301:HOH:O	2.13	0.64
1:A:150:ASP:HB3	1:A:181:LEU:HD13	1.79	0.64
2:H:119:PRO:O	4:H:302:HOH:O	2.15	0.64
2:H:108:ARG:HG3	2:H:108:ARG:HH11	1.60	0.64
1:E:129:PRO:O	4:E:302:HOH:O	2.14	0.64
2:D:4:MET:HE3	2:D:23:CYS:SG	2.37	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:VAL:HG22	1:C:188:VAL:HB	1.80	0.63
1:A:222:CYS:HG	2:B:214:CYS:CB	2.10	0.63
2:B:137:ASN:O	4:B:302:HOH:O	2.15	0.63
3:P:61:GLN:HG3	3:P:66:LEU:HD11	1.79	0.62
2:B:105:GLU:HG3	2:B:173:TYR:OH	1.99	0.62
1:E:142:ALA:N	4:E:301:HOH:O	2.26	0.62
2:B:213:GLU:OE2	2:B:214:CYS:N	2.33	0.62
2:D:142:ARG:HG3	2:D:173:TYR:CD1	2.35	0.61
1:A:222:CYS:CB	2:B:214:CYS:SG	2.90	0.60
3:J:103:THR:HG23	3:J:125:GLU:HA	1.84	0.60
1:C:37:VAL:HG21	1:C:106:MET:HE1	1.82	0.60
3:M:64:GLN:NE2	4:M:201:HOH:O	2.20	0.59
1:G:105:THR:HG21	2:H:34:ALA:HB2	1.84	0.59
2:B:4:MET:HE3	2:B:23:CYS:SG	2.42	0.59
2:F:136:LEU:HD11	2:F:196:VAL:HG21	1.83	0.59
2:F:3:VAL:HG12	2:F:5:THR:HG23	1.85	0.58
1:E:37:VAL:HG22	1:E:47:TRP:HA	1.86	0.58
1:G:125:PRO:HB3	1:G:151:TYR:HB3	1.86	0.58
1:E:100:THR:HG22	1:E:107:ASP:HB3	1.84	0.58
2:B:13:VAL:HG21	2:B:19:ALA:HB2	1.86	0.58
3:P:57:VAL:HG21	3:P:91:LEU:HD13	1.85	0.57
2:D:14:SER:HB2	2:D:17:GLU:HG3	1.87	0.57
1:C:100:THR:HB	1:C:102:TYR:CD2	2.40	0.57
2:D:140:TYR:CD1	2:D:141:PRO:HA	2.39	0.57
2:B:120:PRO:HB3	2:B:131:SER:H	1.68	0.57
1:E:125:PRO:HB3	1:E:151:TYR:HB3	1.87	0.57
3:P:83:ASP:HB3	3:P:84:ARG:HG3	1.87	0.56
3:P:124:LEU:HD12	3:P:125:GLU:N	2.21	0.56
1:A:175:VAL:HG21	2:B:160:GLN:HG2	1.87	0.56
1:A:35:TYR:CE2	1:A:106:MET:HG2	2.40	0.56
2:H:80:SER:O	2:H:83:PHE:HD2	1.89	0.56
2:D:13:VAL:HB	2:D:78:LEU:HD22	1.88	0.56
3:M:112:THR:OG1	3:M:116:GLY:N	2.39	0.56
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.86	0.56
1:C:100:THR:HB	1:C:102:TYR:HD2	1.71	0.56
1:G:179:SER:HB3	1:G:181:LEU:CD1	2.33	0.56
3:J:59:TRP:CD1	3:J:93:LEU:HD13	2.41	0.56
1:E:34:MET:HB3	1:E:79:LEU:HD22	1.88	0.55
3:J:33:ILE:HG12	3:J:41:ILE:HD11	1.89	0.55
3:J:84:ARG:NH2	3:J:102:ASP:OD2	2.37	0.55
2:B:95:PRO:O	2:B:97:THR:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:105:GLU:HG3	2:D:173:TYR:OH	2.07	0.55
2:B:201:LEU:HB2	4:B:315:HOH:O	2.06	0.55
2:B:136:LEU:HB2	2:B:175:LEU:HB3	1.89	0.55
2:B:167:ASP:OD1	2:B:169:LYS:HG2	2.06	0.55
1:G:35:TYR:HB2	1:G:97:ALA:HB3	1.88	0.54
1:E:3:GLN:OE1	1:E:3:GLN:HA	2.07	0.54
2:B:13:VAL:HB	2:B:78:LEU:HD22	1.89	0.54
2:D:24:LYS:HE2	2:D:24:LYS:O	2.07	0.54
1:A:6:GLU:HA	1:A:21:SER:O	2.07	0.54
1:G:1:GLU:C	1:G:26:GLY:HA3	2.32	0.54
2:H:208:SER:O	4:H:303:HOH:O	2.19	0.54
1:G:69:THR:HB	1:G:82:GLN:HB3	1.88	0.54
2:H:105:GLU:OE2	2:H:140:TYR:HE1	1.91	0.54
2:H:119:PRO:HB3	2:H:209:PHE:CZ	2.42	0.54
2:B:149:LYS:HD2	2:B:195:GLU:HB2	1.90	0.54
1:E:150:ASP:OD1	1:E:177:GLN:NE2	2.25	0.54
3:P:124:LEU:HD12	3:P:125:GLU:H	1.73	0.54
3:J:84:ARG:HH22	3:J:102:ASP:CG	2.16	0.54
3:I:99:THR:HG22	3:I:101:ASN:H	1.72	0.53
1:C:6:GLU:HA	1:C:21:SER:O	2.09	0.53
2:F:39:LYS:NZ	4:F:302:HOH:O	2.39	0.53
2:D:124:GLN:O	2:D:127:SER:HB3	2.09	0.53
1:A:105:THR:HG23	2:B:91:TYR:CG	2.44	0.53
2:D:121:SER:OG	2:D:124:GLN:N	2.39	0.53
1:A:160:TRP:CH2	1:A:202:CYS:HB3	2.44	0.53
1:C:201:ILE:CG2	1:C:214:ASP:HB3	2.39	0.53
1:A:156:VAL:CG2	1:A:184:LEU:HD21	2.39	0.53
2:B:183:LYS:O	2:B:187:GLU:HG3	2.09	0.53
2:F:54:ARG:CZ	2:F:60:ALA:HA	2.39	0.52
2:B:169:LYS:NZ	4:B:304:HOH:O	2.24	0.52
1:E:204:VAL:HB	1:E:213:VAL:HG13	1.91	0.52
1:A:169:VAL:HG22	1:A:188:VAL:HB	1.92	0.52
1:G:209:SER:HB2	1:G:211:THR:HG23	1.91	0.52
2:H:120:PRO:HD3	2:H:132:VAL:HG22	1.92	0.52
2:B:113:PRO:HB3	2:B:139:PHE:HB3	1.92	0.52
1:C:20:LEU:HD12	1:C:81:LEU:HD23	1.91	0.52
1:C:176:LEU:O	2:D:160:GLN:NE2	2.42	0.52
2:D:28:ASP:OD2	2:D:68:GLY:HA2	2.09	0.52
1:E:39:GLN:HG3	1:E:44:GLY:O	2.09	0.52
1:C:104:PHE:CE1	3:J:78:SER:HB2	2.45	0.51
1:A:105:THR:CG2	2:B:91:TYR:CD2	2.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:ILE:CG2	1:A:214:ASP:HB3	2.40	0.51
1:G:9:GLY:HA2	1:G:18:LEU:HD21	1.91	0.51
1:A:163:GLY:O	4:A:301:HOH:O	2.18	0.51
1:E:199:THR:HG23	1:E:216:LYS:HE3	1.92	0.51
2:D:33:VAL:HG21	2:D:71:PHE:CE2	2.45	0.51
2:D:136:LEU:HD11	2:D:146:VAL:HG23	1.93	0.51
1:C:206:HIS:ND1	1:C:209:SER:HB3	2.26	0.50
1:G:105:THR:HG23	2:H:91:TYR:CD2	2.46	0.50
1:A:73:ASP:OD1	1:A:76:LYS:HG3	2.12	0.50
1:C:7:SER:HB3	4:C:318:HOH:O	2.11	0.50
3:J:33:ILE:HG22	3:J:34:SER:N	2.26	0.50
3:P:73:LEU:HD13	2:H:50:TRP:CG	2.46	0.50
2:F:46:LEU:HD23	2:F:55:HIS:ND1	2.26	0.50
1:G:34:MET:HB3	1:G:79:LEU:HD22	1.93	0.50
1:A:35:TYR:CD2	1:A:106:MET:HG2	2.46	0.50
2:F:120:PRO:HD3	2:F:132:VAL:HG22	1.92	0.50
1:G:3:GLN:O	1:G:24:ALA:HA	2.12	0.50
2:H:18:ARG:HG2	2:H:76:SER:HA	1.93	0.50
2:B:182:SER:HB2	2:B:185:ASP:H	1.76	0.50
1:C:83:MET:HE2	1:C:86:LEU:HD21	1.94	0.50
1:E:47:TRP:NE1	1:E:49:ALA:O	2.42	0.50
2:D:179:LEU:CD2	2:D:181:LEU:HD11	2.42	0.50
1:E:33:TYR:CD1	1:E:52:THR:HA	2.47	0.50
2:H:108:ARG:HG3	2:H:108:ARG:NH1	2.27	0.49
2:H:149:LYS:HG2	2:H:154:LEU:HG	1.94	0.49
2:B:35:TRP:CD2	2:B:73:LEU:HB2	2.47	0.49
3:M:23:MET:O	3:M:23:MET:HG3	2.12	0.49
3:P:50:THR:OG1	3:P:52:ALA:N	2.41	0.49
1:G:174:ALA:HA	1:G:184:LEU:HB3	1.94	0.49
3:J:27:ILE:HG21	3:J:120:GLY:HA3	1.94	0.49
1:G:1:GLU:O	1:G:26:GLY:HA3	2.13	0.49
1:G:220:LYS:NZ	4:H:301:HOH:O	2.26	0.49
2:D:213:GLU:HG3	2:D:214:CYS:H	1.77	0.49
2:H:18:ARG:NH2	2:H:74:THR:CG2	2.72	0.49
1:A:70:ILE:O	4:A:303:HOH:O	2.20	0.49
1:C:64:VAL:HG13	1:C:68:PHE:CG	2.48	0.48
1:E:37:VAL:O	1:E:95:TYR:HB2	2.13	0.48
2:F:11:LEU:HB3	2:F:104:VAL:HG23	1.95	0.48
2:B:161:GLU:HG2	2:B:175:LEU:HD11	1.95	0.48
1:C:201:ILE:HG21	1:C:214:ASP:HB3	1.95	0.48
2:D:46:LEU:HD23	2:D:55:HIS:CD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:191:VAL:HG12	2:F:210:ASN:OD1	2.13	0.48
1:G:129:PRO:O	4:G:302:HOH:O	2.20	0.48
1:G:154:GLU:OE1	1:G:155:PRO:HA	2.14	0.48
1:G:177:GLN:HB2	1:G:179:SER:HB2	1.95	0.48
2:D:94:TYR:CZ	3:J:79:PRO:HB2	2.49	0.48
2:F:32:SER:HB3	2:F:91:TYR:CD1	2.49	0.48
3:P:77:ILE:HD11	3:P:87:PRO:HG3	1.94	0.48
1:C:6:GLU:OE1	1:C:6:GLU:N	2.44	0.48
2:H:89:GLN:HG2	2:H:90:GLN:N	2.29	0.48
1:E:64:VAL:HG13	1:E:68:PHE:CG	2.49	0.48
3:P:58:ASN:HB2	3:P:109:ILE:HB	1.96	0.48
2:B:105:GLU:OE1	2:B:106:ILE:O	2.32	0.47
1:C:150:ASP:HB3	1:C:181:LEU:HD12	1.95	0.47
2:F:119:PRO:HB3	2:F:209:PHE:CE1	2.48	0.47
1:E:20:LEU:HG	1:E:83:MET:HE2	1.95	0.47
2:F:24:LYS:HG3	4:F:310:HOH:O	2.14	0.47
2:F:117:ILE:HD12	2:F:194:CYS:HB2	1.94	0.47
3:I:99:THR:CG2	3:I:101:ASN:HD22	2.26	0.47
3:I:99:THR:HG22	3:I:101:ASN:HD22	1.80	0.47
2:D:13:VAL:HG21	2:D:19:ALA:HB2	1.97	0.47
3:P:27:ILE:HA	3:P:46:HIS:O	2.15	0.47
1:C:67:ARG:NH1	1:C:90:ASP:OD2	2.47	0.47
1:G:64:VAL:HA	1:G:67:ARG:NH2	2.29	0.47
1:C:39:GLN:HG3	1:C:44:GLY:O	2.15	0.47
1:E:67:ARG:HH12	1:E:90:ASP:CG	2.23	0.47
2:F:7:SER:HB3	2:F:22:SER:O	2.14	0.47
1:G:23:ALA:HA	1:G:78:THR:HG22	1.97	0.47
1:A:71:SER:O	1:A:79:LEU:HD12	2.15	0.46
2:D:80:SER:HA	2:D:106:ILE:HD12	1.97	0.46
1:A:105:THR:HG23	2:B:91:TYR:CD2	2.50	0.46
1:A:201:ILE:HG21	1:A:214:ASP:HB3	1.97	0.46
2:B:206:THR:OG1	4:B:303:HOH:O	2.20	0.46
1:C:35:TYR:CE1	1:C:50:TYR:HD2	2.34	0.46
2:F:187:GLU:OE1	4:F:301:HOH:O	2.20	0.46
1:E:71:SER:O	1:E:79:LEU:HD12	2.15	0.46
2:D:54:ARG:HD2	2:D:58:ILE:O	2.15	0.46
1:C:36:TRP:NE1	1:C:81:LEU:HB2	2.30	0.46
2:D:35:TRP:CZ3	2:D:88:CYS:HB3	2.50	0.46
3:M:40:SER:HA	3:M:95:LEU:O	2.15	0.46
1:E:216:LYS:HD3	1:E:218:GLU:OE1	2.15	0.46
3:J:27:ILE:HD11	3:J:118:TYR:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:175:LEU:HD23	2:H:176:SER:N	2.30	0.46
2:F:13:VAL:CG1	2:F:17:GLU:HB3	2.45	0.46
2:F:37:GLN:HB2	2:F:47:LEU:HD11	1.96	0.46
3:I:113:TYR:CD1	3:I:114:PRO:HA	2.51	0.46
1:A:104:PHE:CE2	3:I:78:SER:HB2	2.50	0.46
1:E:83:MET:HE1	1:E:115:VAL:HG21	1.98	0.46
2:B:33:VAL:HG21	2:B:71:PHE:CE2	2.50	0.45
2:D:150:VAL:HB	2:D:155:GLN:NE2	2.31	0.45
1:G:105:THR:HG23	2:H:91:TYR:CE2	2.51	0.45
2:D:134:CYS:HB2	2:D:148:TRP:CZ2	2.51	0.45
3:I:110:TYR:O	3:I:117:THR:HA	2.16	0.45
1:C:104:PHE:CD1	3:J:78:SER:HB2	2.52	0.45
2:D:59:PRO:HB2	2:D:61:ARG:HG2	1.98	0.45
2:F:6:GLN:HG2	2:F:23:CYS:HB2	1.99	0.45
2:F:84:ALA:H	2:F:104:VAL:HG12	1.81	0.45
3:J:33:ILE:HG21	3:J:41:ILE:CD1	2.44	0.45
3:M:125:GLU:CD	3:M:127:LEU:HD21	2.40	0.45
3:P:93:LEU:HD12	3:P:93:LEU:HA	1.67	0.45
1:A:105:THR:HG21	2:B:91:TYR:CD2	2.51	0.45
1:A:160:TRP:CZ3	1:A:202:CYS:HB3	2.52	0.45
1:C:149:LYS:HG2	1:C:150:ASP:CG	2.42	0.45
2:F:151:ASP:HA	2:F:191:VAL:CG2	2.46	0.45
1:G:102:TYR:HD1	2:H:49:TYR:CE2	2.34	0.45
2:F:136:LEU:HD11	2:F:196:VAL:CG2	2.45	0.45
2:F:142:ARG:HD2	2:F:163:VAL:HG21	1.98	0.45
2:F:198:HIS:ND1	2:F:199:GLN:N	2.63	0.45
3:P:103:THR:HG23	3:P:125:GLU:HA	1.98	0.45
1:A:33:TYR:HD2	1:A:52:THR:HA	1.82	0.45
1:A:120:ALA:HB3	1:A:152:PHE:CE2	2.52	0.45
2:B:130:ALA:O	2:B:180:THR:HA	2.17	0.45
2:F:22:SER:OG	2:F:23:CYS:N	2.49	0.45
1:G:105:THR:HB	1:G:106:MET:H	1.55	0.45
1:A:31:ASP:O	1:A:53:LYS:HE2	2.17	0.45
2:F:4:MET:HE1	2:F:25:ALA:HB2	1.98	0.45
2:F:145:LYS:HB2	2:F:197:THR:CG2	2.47	0.45
2:H:37:GLN:HB2	2:H:86:TYR:CE2	2.51	0.45
3:M:44:GLN:HG3	3:M:92:GLY:HA3	1.98	0.45
2:D:136:LEU:HD21	2:D:196:VAL:HG21	1.97	0.44
1:E:11:LEU:HD12	1:E:116:THR:O	2.16	0.44
3:P:41:ILE:HD12	3:P:41:ILE:HA	1.81	0.44
1:C:105:THR:HB	2:D:91:TYR:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:98:ARG:O	1:G:106:MET:HA	2.16	0.44
1:E:130:LEU:HB3	2:F:118:PHE:CD1	2.52	0.44
1:C:76:LYS:O	1:C:78:THR:HG23	2.18	0.44
2:D:108:ARG:HG3	2:D:140:TYR:CD2	2.53	0.44
2:D:167:ASP:O	2:D:168:SER:HB3	2.17	0.44
1:G:220:LYS:HG3	4:G:318:HOH:O	2.18	0.44
1:C:222:CYS:HB3	2:D:214:CYS:SG	2.58	0.44
2:F:119:PRO:HB3	2:F:209:PHE:CZ	2.52	0.44
3:J:40:SER:HB3	3:J:96:GLN:HA	2.00	0.44
1:C:222:CYS:CB	2:D:214:CYS:HG	2.29	0.44
3:J:61:GLN:O	3:J:62:GLN:HB3	2.18	0.44
1:A:51:ILE:HG13	1:A:58:THR:HG22	2.00	0.44
3:J:27:ILE:HG21	3:J:120:GLY:CA	2.48	0.44
2:H:78:LEU:HD23	2:H:78:LEU:HA	1.79	0.44
1:A:57:SER:HA	4:A:331:HOH:O	2.17	0.44
3:I:57:VAL:HA	3:I:109:ILE:O	2.18	0.44
3:P:27:ILE:HG23	3:P:46:HIS:O	2.18	0.44
1:E:67:ARG:O	1:E:84:ASN:HB2	2.18	0.43
2:D:106:ILE:HG22	2:D:166:GLN:OE1	2.18	0.43
3:I:77:ILE:HD12	3:I:85:VAL:HG12	2.01	0.43
1:A:27:PHE:CE2	1:A:29:PHE:HA	2.53	0.43
1:A:36:TRP:HB2	1:A:49:ALA:HB3	2.01	0.43
1:A:126:SER:N	4:A:302:HOH:O	2.50	0.43
2:B:190:LYS:HE3	2:B:210:ASN:HB3	2.00	0.43
1:C:30:SER:HB2	4:C:313:HOH:O	2.17	0.43
1:C:191:PRO:O	1:C:194:SER:HB3	2.18	0.43
2:F:8:PRO:HD3	4:F:338:HOH:O	2.19	0.43
2:F:125:LEU:HD23	2:F:125:LEU:HA	1.74	0.43
3:M:59:TRP:CG	3:M:93:LEU:HD22	2.53	0.43
1:G:133:SER:OG	1:G:134:SER:N	2.51	0.43
1:A:35:TYR:CD1	1:A:50:TYR:HD2	2.35	0.43
2:B:119:PRO:HB3	2:B:209:PHE:CE1	2.54	0.43
1:C:27:PHE:CE2	1:C:29:PHE:HA	2.53	0.43
1:E:91:THR:O	4:E:303:HOH:O	2.21	0.43
2:F:151:ASP:HA	2:F:191:VAL:HG23	1.99	0.43
1:G:110:GLY:O	2:H:43:ALA:HB2	2.18	0.43
2:D:55:HIS:ND1	2:D:56:THR:O	2.50	0.43
1:G:128:PHE:CE2	2:H:124:GLN:HG3	2.54	0.43
2:H:75:ILE:HD12	2:H:78:LEU:HD21	2.01	0.43
1:A:176:LEU:HD12	1:A:182:TYR:CE2	2.54	0.43
2:B:145:LYS:HA	2:B:145:LYS:HD3	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:ASN:HB2	4:C:305:HOH:O	2.18	0.43
2:D:183:LYS:O	2:D:187:GLU:HG3	2.18	0.43
1:E:33:TYR:HD1	1:E:52:THR:HA	1.83	0.43
3:M:112:THR:HG21	3:M:118:TYR:CE2	2.54	0.43
1:C:195:LEU:HD23	1:C:195:LEU:HA	1.83	0.43
1:E:57:SER:HB3	1:E:59:TYR:HE2	1.84	0.43
2:F:11:LEU:HD23	2:F:11:LEU:HA	1.75	0.43
1:G:38:ARG:HD3	1:G:48:VAL:HG11	1.99	0.43
1:G:60:TYR:CZ	1:G:70:ILE:HG22	2.54	0.43
2:H:55:HIS:HB3	2:H:58:ILE:HG13	2.01	0.43
1:E:9:GLY:H	1:E:113:THR:HG21	1.84	0.42
1:G:29:PHE:CE1	1:G:34:MET:HG3	2.54	0.42
1:G:47:TRP:CD2	2:H:96:LEU:HD12	2.54	0.42
2:D:161:GLU:CD	2:D:175:LEU:HD11	2.44	0.42
3:M:84:ARG:HH22	3:M:102:ASP:CG	2.28	0.42
3:M:121:ARG:NH1	4:M:202:HOH:O	2.29	0.42
3:P:75:TRP:CD2	3:P:87:PRO:HB3	2.54	0.42
2:H:142:ARG:NH2	2:H:163:VAL:HG21	2.34	0.42
1:A:67:ARG:NH1	1:A:90:ASP:OD2	2.52	0.42
2:D:89:GLN:HB2	2:D:98:PHE:CD2	2.54	0.42
1:G:39:GLN:HB2	1:G:45:LEU:HD23	2.01	0.42
2:H:7:SER:HA	2:H:8:PRO:HA	1.77	0.42
1:C:35:TYR:CE1	1:C:50:TYR:CD2	3.07	0.42
2:D:7:SER:HA	2:D:8:PRO:HA	1.64	0.42
3:I:27:ILE:HG21	3:I:120:GLY:HA3	2.01	0.42
3:P:111:HIS:HA	3:P:116:GLY:O	2.19	0.42
1:E:165:LEU:HD12	1:E:165:LEU:HA	1.79	0.42
1:G:35:TYR:CD2	1:G:106:MET:HG2	2.55	0.42
2:H:154:LEU:H	2:H:154:LEU:HD12	1.85	0.42
1:A:91:THR:HG23	1:A:116:THR:HA	2.02	0.42
1:A:171:THR:HG23	1:A:186:SER:HB2	2.01	0.42
2:B:93:SER:HA	3:I:79:PRO:HB3	2.01	0.42
2:F:78:LEU:HD12	2:F:78:LEU:HA	1.74	0.42
1:G:47:TRP:CG	2:H:96:LEU:HD12	2.55	0.42
1:G:51:ILE:HD13	1:G:72:ARG:HD2	2.01	0.42
2:H:37:GLN:HB2	2:H:47:LEU:HD11	2.01	0.42
2:F:7:SER:OG	2:F:8:PRO:O	2.38	0.42
3:I:109:ILE:HG23	3:I:117:THR:HG23	2.01	0.42
3:M:87:PRO:HA	3:M:93:LEU:HD12	2.02	0.42
3:M:110:TYR:HB2	3:M:118:TYR:HB2	2.01	0.42
2:D:126:LYS:HA	2:D:126:LYS:HD2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:50:THR:HB	3:P:51:THR:H	1.78	0.42
1:E:8:GLY:O	1:E:18:LEU:HD11	2.20	0.42
2:F:145:LYS:HD3	2:F:145:LYS:HA	1.85	0.42
1:C:29:PHE:O	1:C:72:ARG:NH2	2.53	0.42
2:D:184:ALA:HA	4:D:330:HOH:O	2.20	0.42
3:M:41:ILE:HD13	3:M:41:ILE:HA	1.84	0.42
1:A:32:TYR:CD2	1:A:98:ARG:HD2	2.55	0.41
1:E:13:GLN:HG2	4:E:324:HOH:O	2.20	0.41
1:E:195:LEU:HD23	1:E:195:LEU:HA	1.83	0.41
1:G:39:GLN:HG3	1:G:44:GLY:O	2.20	0.41
2:H:91:TYR:CD2	2:H:91:TYR:N	2.88	0.41
2:H:13:VAL:CG1	2:H:17:GLU:HB3	2.47	0.41
1:A:99:GLN:HA	1:A:105:THR:O	2.21	0.41
1:A:101:ASN:ND2	4:A:307:HOH:O	2.53	0.41
2:D:143:GLU:O	2:D:198:HIS:HD2	2.04	0.41
1:E:127:VAL:HG21	1:E:213:VAL:HG11	2.02	0.41
3:J:98:LEU:HD13	3:J:126:VAL:HG22	2.03	0.41
1:G:160:TRP:CZ3	1:G:202:CYS:HB3	2.55	0.41
2:H:183:LYS:O	2:H:187:GLU:HG3	2.21	0.41
3:M:84:ARG:NH2	3:M:102:ASP:OD2	2.54	0.41
1:G:33:TYR:CD1	1:G:52:THR:HA	2.56	0.41
1:G:150:ASP:OD1	1:G:177:GLN:NE2	2.46	0.41
1:C:100:THR:HG23	1:C:105:THR:O	2.21	0.41
2:B:197:THR:HG22	4:B:340:HOH:O	2.21	0.41
1:C:68:PHE:HB3	1:C:81:LEU:HD11	2.02	0.41
1:C:160:TRP:HB3	1:C:165:LEU:HD23	2.02	0.41
1:E:131:ALA:HB3	1:E:220:LYS:HG3	2.03	0.41
1:A:5:VAL:O	1:A:22:CYS:HA	2.20	0.41
1:A:36:TRP:NE1	1:A:81:LEU:HB2	2.35	0.41
1:A:149:LYS:HG2	1:A:150:ASP:OD1	2.21	0.41
1:E:105:THR:HB	2:F:91:TYR:CE2	2.56	0.41
1:G:102:TYR:CD2	1:G:102:TYR:N	2.89	0.41
1:G:13:GLN:HE21	1:G:13:GLN:HB3	1.55	0.41
1:A:12:VAL:HG11	1:A:86:LEU:HD13	2.02	0.40
1:A:83:MET:HE2	1:A:86:LEU:HD21	2.02	0.40
4:E:306:HOH:O	2:F:45:ARG:HA	2.21	0.40
1:G:205:ASN:OD1	1:G:212:LYS:HG2	2.21	0.40
3:P:44:GLN:HG3	3:P:45:CYS:N	2.36	0.40
1:G:29:PHE:HE1	1:G:34:MET:HG3	1.86	0.40
1:A:60:TYR:CE1	1:A:70:ILE:HG22	2.57	0.40
2:D:179:LEU:HD23	2:D:181:LEU:HD11	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:87:ARG:HH11	1:E:87:ARG:HD2	1.76	0.40
2:F:83:PHE:HA	2:F:104:VAL:HG13	2.04	0.40
2:F:148:TRP:CE2	2:F:179:LEU:HB2	2.56	0.40
3:I:62:GLN:HG2	3:I:105:GLU:HB2	2.03	0.40
1:G:152:PHE:HA	1:G:153:PRO:HA	1.89	0.40
1:C:50:TYR:HD1	1:C:59:TYR:CD2	2.39	0.40
3:I:99:THR:HG22	3:I:100:VAL:N	2.36	0.40
3:P:40:SER:HA	3:P:95:LEU:O	2.22	0.40
1:G:47:TRP:O	1:G:61:PRO:HG3	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:336:HOH:O	4:G:308:HOH:O[1_455]	2.19	0.01
3:J:44:GLN:NE2	3:P:44:GLN:OE1[2_545]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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	213/222 (96%)	199 (93%)	14 (7%)	0	100	100
1	C	213/222 (96%)	201 (94%)	11 (5%)	1 (0%)	24	46
1	E	213/222 (96%)	205 (96%)	8 (4%)	0	100	100
1	G	213/222 (96%)	196 (92%)	16 (8%)	1 (0%)	24	46
2	B	212/214 (99%)	206 (97%)	6 (3%)	0	100	100
2	D	212/214 (99%)	201 (95%)	11 (5%)	0	100	100
2	F	212/214 (99%)	202 (95%)	9 (4%)	1 (0%)	24	46
2	H	212/214 (99%)	205 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	I	104/115 (90%)	101 (97%)	3 (3%)	0	100	100
3	J	104/115 (90%)	99 (95%)	5 (5%)	0	100	100
3	M	104/115 (90%)	94 (90%)	8 (8%)	2 (2%)	6	15
3	P	102/115 (89%)	93 (91%)	8 (8%)	1 (1%)	12	30
All	All	2114/2204 (96%)	2002 (95%)	106 (5%)	6 (0%)	36	59

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	7	SER
3	P	114	PRO
3	M	117	THR
1	G	64	VAL
3	M	114	PRO
1	C	153	PRO

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	182/186 (98%)	182 (100%)	0	100	100
1	C	182/186 (98%)	182 (100%)	0	100	100
1	E	182/186 (98%)	182 (100%)	0	100	100
1	G	182/186 (98%)	181 (100%)	1 (0%)	81	91
2	B	184/184 (100%)	184 (100%)	0	100	100
2	D	184/184 (100%)	184 (100%)	0	100	100
2	F	184/184 (100%)	184 (100%)	0	100	100
2	H	184/184 (100%)	184 (100%)	0	100	100
3	I	90/99 (91%)	90 (100%)	0	100	100
3	J	90/99 (91%)	90 (100%)	0	100	100
3	M	90/99 (91%)	90 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	P	88/99 (89%)	88 (100%)	0	100	100
All	All	1822/1876 (97%)	1821 (100%)	1 (0%)	88	95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	67	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	74	ASN
2	D	137	ASN
1	E	77	ASN
2	F	79	GLN
2	F	138	ASN
2	F	160	GLN
3	I	44	GLN
3	I	101	ASN
3	J	56	GLN
3	J	62	GLN
3	J	64	GLN
3	J	70	ASN
3	M	53	GLN
3	M	96	GLN
3	P	62	GLN
1	G	13	GLN
1	G	101	ASN
1	G	170	HIS
1	G	198	GLN
2	H	55	HIS
2	H	138	ASN
2	H	147	GLN
2	H	210	ASN

5.3.3 RNA ⓘ

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](#)

There are no ligands in this entry.

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	217/222 (97%)	0.38	1 (0%) 87 86	31, 44, 65, 108	0
1	C	217/222 (97%)	0.44	8 (3%) 45 41	31, 45, 72, 109	0
1	E	217/222 (97%)	0.47	2 (0%) 81 80	33, 46, 61, 109	0
1	G	217/222 (97%)	0.56	7 (3%) 50 47	35, 49, 63, 117	0
2	B	214/214 (100%)	0.43	4 (1%) 66 63	29, 44, 60, 105	0
2	D	214/214 (100%)	0.43	6 (2%) 55 52	31, 47, 61, 91	0
2	F	214/214 (100%)	0.47	4 (1%) 66 63	32, 43, 56, 103	0
2	H	214/214 (100%)	0.60	5 (2%) 61 58	35, 47, 60, 102	0
3	I	106/115 (92%)	0.58	3 (2%) 55 52	31, 43, 57, 70	0
3	J	106/115 (92%)	0.53	2 (1%) 66 63	31, 47, 65, 78	0
3	M	106/115 (92%)	0.77	11 (10%) 11 10	36, 48, 79, 88	0
3	P	104/115 (90%)	0.71	9 (8%) 16 14	37, 48, 75, 100	0
All	All	2146/2204 (97%)	0.51	62 (2%) 53 50	29, 46, 64, 117	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	P	51	THR	5.4
3	M	116	GLY	5.2
3	M	117	THR	3.8
2	F	214	CYS	3.6
2	H	13	VAL	3.5
2	B	214	CYS	3.3
1	E	140	GLY	3.3
1	A	222	CYS	3.2
3	P	25	GLY	3.1
3	P	50	THR	3.1
1	C	102	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
3	I	96	GLN	3.0
3	J	23	MET	3.0
3	I	24	THR	2.9
3	M	52	ALA	2.9
1	G	108	TYR	2.9
3	P	52	ALA	2.9
2	F	7	SER	2.8
1	C	101	ASN	2.7
1	C	134	SER	2.7
3	M	23	MET	2.7
2	F	13	VAL	2.6
1	G	1	GLU	2.6
1	G	140	GLY	2.6
1	G	220	LYS	2.6
2	B	129	THR	2.5
3	P	122	ILE	2.5
3	P	62	GLN	2.4
3	M	24	THR	2.4
2	D	168	SER	2.4
3	P	124	LEU	2.4
2	F	162	SER	2.4
2	D	181	LEU	2.3
2	H	34	ALA	2.3
3	M	112	THR	2.3
2	D	18	ARG	2.3
2	D	70	GLU	2.3
1	C	219	PRO	2.3
3	M	114	PRO	2.3
2	H	82	ASP	2.3
2	H	154	LEU	2.3
1	G	111	GLN	2.2
2	H	12	SER	2.2
2	D	126	LYS	2.2
3	M	54	VAL	2.2
3	I	128	GLU	2.1
1	C	222	CYS	2.1
1	C	213	VAL	2.1
1	G	64	VAL	2.1
3	M	51	THR	2.1
3	P	61	GLN	2.1
2	B	128	GLY	2.1
1	E	221	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	184	ALA	2.1
3	J	24	THR	2.1
2	D	11	LEU	2.1
3	M	41	ILE	2.1
3	P	115	ASP	2.0
1	G	221	SER	2.0
1	C	202	CYS	2.0
3	M	113	TYR	2.0
1	C	221	SER	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.