



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:16 PM GMT

PDB ID : 3TCF
Title : Crystal structure of E. coli OppA complexed with endogenous ligands
Authors : Klepsch, M.M.; Kovermann, M.; Low, C.; Balbach, J.; de Gier, J.W.; Slotboom, D.J.; Berntsson, R.P.-A.
Deposited on : 2011-08-09
Resolution : 2.00 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

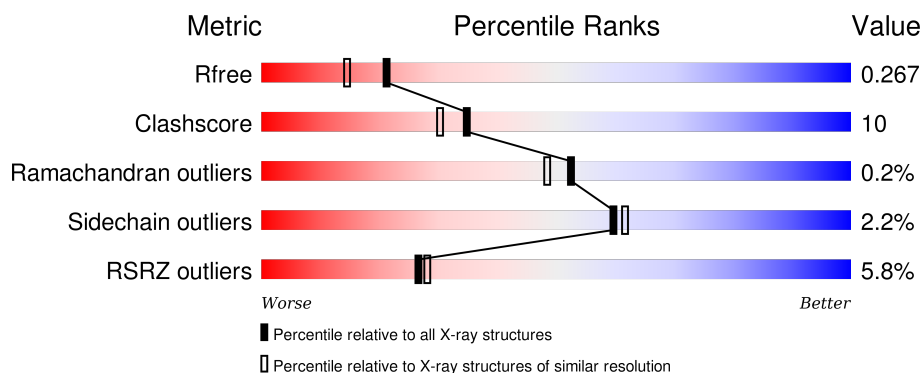
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	524	
1	B	524	
1	C	524	
1	D	524	
1	E	524	

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Mol	Chain	Length	Quality of chain
1	F	524	
1	G	524	
1	H	524	
2	I	3	
2	J	3	
2	K	3	
2	L	3	
2	M	3	
2	N	3	
2	O	3	
2	P	3	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 35615 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 Periplasmic oligopeptide-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	517	Total	C	N	O	S	0	2	0
			4137	2636	695	796	10			
1	B	517	Total	C	N	O	S	0	2	0
			4136	2636	694	796	10			
1	C	517	Total	C	N	O	S	0	1	0
			4129	2632	693	794	10			
1	D	517	Total	C	N	O	S	0	1	0
			4129	2632	693	794	10			
1	E	517	Total	C	N	O	S	0	2	0
			4137	2636	694	797	10			
1	F	517	Total	C	N	O	S	0	4	0
			4155	2649	696	800	10			
1	G	517	Total	C	N	O	S	0	2	0
			4135	2635	694	796	10			
1	H	517	Total	C	N	O	S	0	1	0
			4129	2632	693	794	10			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	MET	-	EXPRESSION TAG	UNP P23843
A	544	HIS	-	EXPRESSION TAG	UNP P23843
A	545	HIS	-	EXPRESSION TAG	UNP P23843
A	546	HIS	-	EXPRESSION TAG	UNP P23843
A	547	HIS	-	EXPRESSION TAG	UNP P23843
A	548	HIS	-	EXPRESSION TAG	UNP P23843
A	549	HIS	-	EXPRESSION TAG	UNP P23843
B	26	MET	-	EXPRESSION TAG	UNP P23843
B	544	HIS	-	EXPRESSION TAG	UNP P23843
B	545	HIS	-	EXPRESSION TAG	UNP P23843
B	546	HIS	-	EXPRESSION TAG	UNP P23843
B	547	HIS	-	EXPRESSION TAG	UNP P23843
B	548	HIS	-	EXPRESSION TAG	UNP P23843

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Chain	Residue	Modelled	Actual	Comment	Reference
B	549	HIS	-	EXPRESSION TAG	UNP P23843
C	26	MET	-	EXPRESSION TAG	UNP P23843
C	544	HIS	-	EXPRESSION TAG	UNP P23843
C	545	HIS	-	EXPRESSION TAG	UNP P23843
C	546	HIS	-	EXPRESSION TAG	UNP P23843
C	547	HIS	-	EXPRESSION TAG	UNP P23843
C	548	HIS	-	EXPRESSION TAG	UNP P23843
C	549	HIS	-	EXPRESSION TAG	UNP P23843
D	26	MET	-	EXPRESSION TAG	UNP P23843
D	544	HIS	-	EXPRESSION TAG	UNP P23843
D	545	HIS	-	EXPRESSION TAG	UNP P23843
D	546	HIS	-	EXPRESSION TAG	UNP P23843
D	547	HIS	-	EXPRESSION TAG	UNP P23843
D	548	HIS	-	EXPRESSION TAG	UNP P23843
D	549	HIS	-	EXPRESSION TAG	UNP P23843
E	26	MET	-	EXPRESSION TAG	UNP P23843
E	544	HIS	-	EXPRESSION TAG	UNP P23843
E	545	HIS	-	EXPRESSION TAG	UNP P23843
E	546	HIS	-	EXPRESSION TAG	UNP P23843
E	547	HIS	-	EXPRESSION TAG	UNP P23843
E	548	HIS	-	EXPRESSION TAG	UNP P23843
E	549	HIS	-	EXPRESSION TAG	UNP P23843
F	26	MET	-	EXPRESSION TAG	UNP P23843
F	544	HIS	-	EXPRESSION TAG	UNP P23843
F	545	HIS	-	EXPRESSION TAG	UNP P23843
F	546	HIS	-	EXPRESSION TAG	UNP P23843
F	547	HIS	-	EXPRESSION TAG	UNP P23843
F	548	HIS	-	EXPRESSION TAG	UNP P23843
F	549	HIS	-	EXPRESSION TAG	UNP P23843
G	26	MET	-	EXPRESSION TAG	UNP P23843
G	544	HIS	-	EXPRESSION TAG	UNP P23843
G	545	HIS	-	EXPRESSION TAG	UNP P23843
G	546	HIS	-	EXPRESSION TAG	UNP P23843
G	547	HIS	-	EXPRESSION TAG	UNP P23843
G	548	HIS	-	EXPRESSION TAG	UNP P23843
G	549	HIS	-	EXPRESSION TAG	UNP P23843
H	26	MET	-	EXPRESSION TAG	UNP P23843
H	544	HIS	-	EXPRESSION TAG	UNP P23843
H	545	HIS	-	EXPRESSION TAG	UNP P23843
H	546	HIS	-	EXPRESSION TAG	UNP P23843
H	547	HIS	-	EXPRESSION TAG	UNP P23843
H	548	HIS	-	EXPRESSION TAG	UNP P23843

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Chain	Residue	Modelled	Actual	Comment	Reference
H	549	HIS	-	EXPRESSION TAG	UNP P23843

- Molecule 2 is a protein called Endogenous peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	3	Total	C	N	O	0	0	0
			15	9	3	3			
2	J	3	Total	C	N	O	0	0	0
			15	9	3	3			
2	K	3	Total	C	N	O	0	0	0
			15	9	3	3			
2	L	3	Total	C	N	O	0	0	0
			15	9	3	3			
2	M	3	Total	C	N	O	0	0	0
			15	9	3	3			
2	N	3	Total	C	N	O	0	0	0
			15	9	3	3			
2	O	3	Total	C	N	O	0	0	0
			15	9	3	3			
2	P	3	Total	C	N	O	0	0	0
			15	9	3	3			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	360	Total	O	0	0
			360	360		
3	B	268	Total	O	0	0
			268	268		
3	C	285	Total	O	0	0
			285	285		
3	D	265	Total	O	0	0
			265	265		
3	E	351	Total	O	0	0
			351	351		
3	F	344	Total	O	0	0
			344	344		
3	G	305	Total	O	0	0
			305	305		
3	H	221	Total	O	0	0
			221	221		
3	I	2	Total	O	0	0
			2	2		

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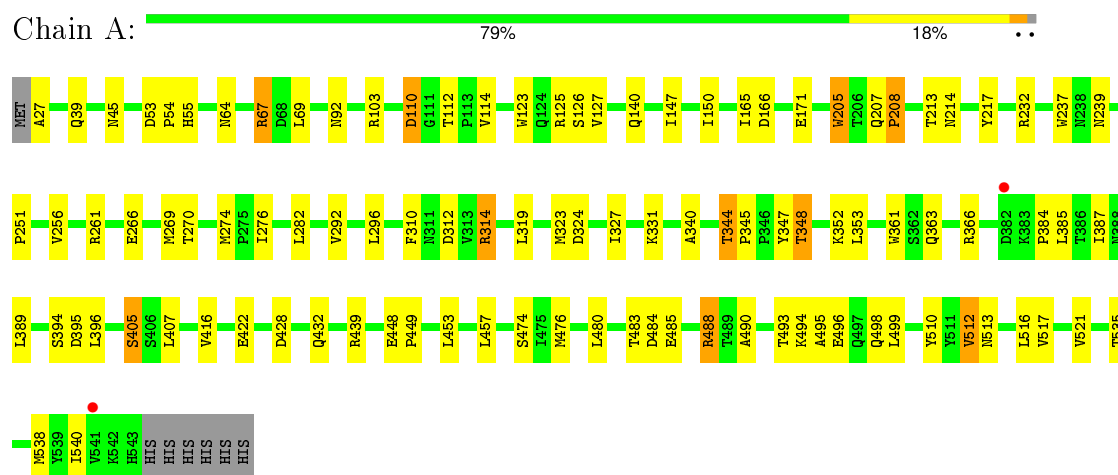
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	2	Total	O	0	0
			2	2		
3	K	1	Total	O	0	0
			1	1		
3	M	2	Total	O	0	0
			2	2		
3	P	2	Total	O	0	0
			2	2		

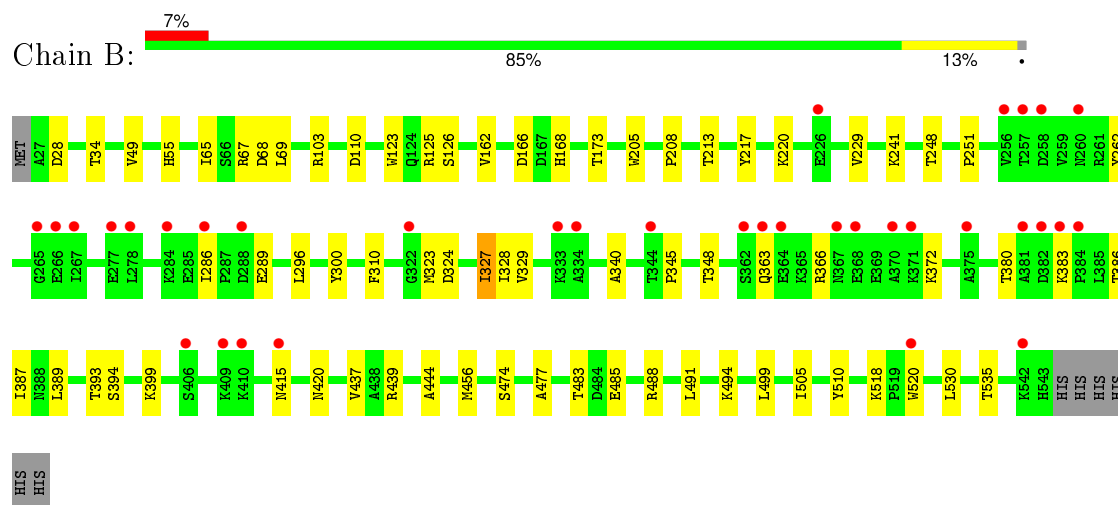
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

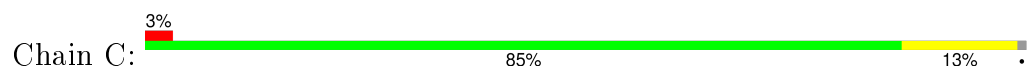
• Molecule 1: Periplasmic oligopeptide-binding protein

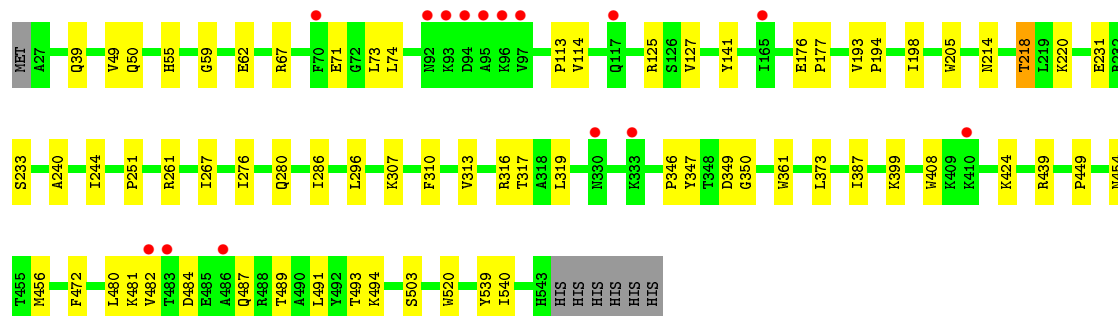


• Molecule 1: Periplasmic oligopeptide-binding protein

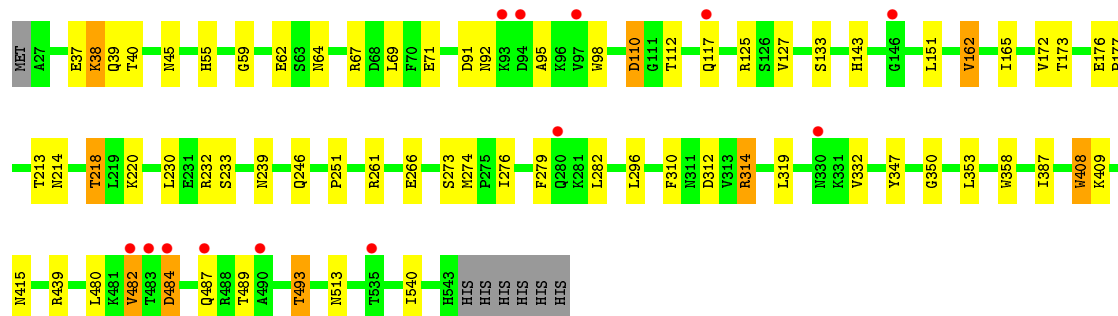
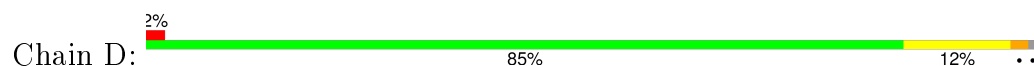


• Molecule 1: Periplasmic oligopeptide-binding protein

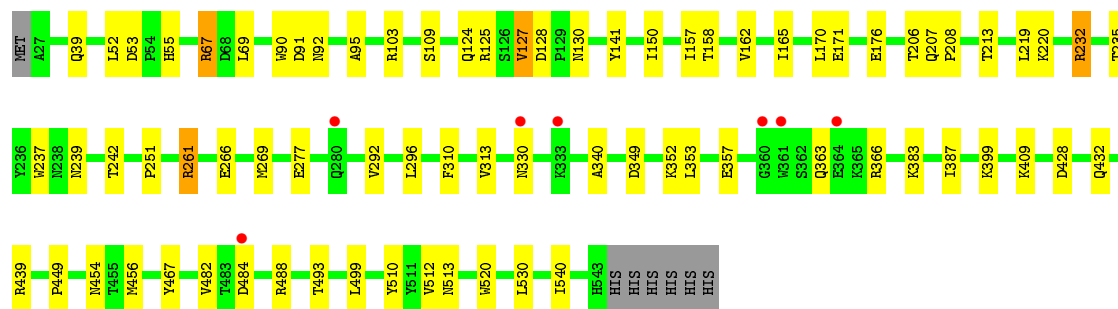
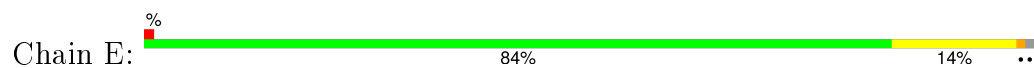




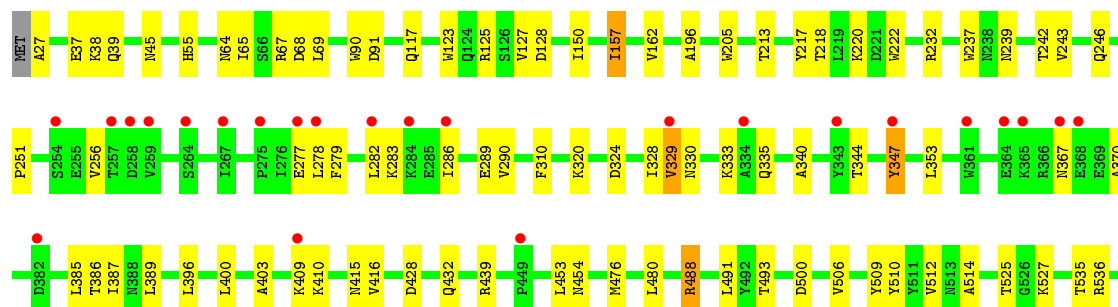
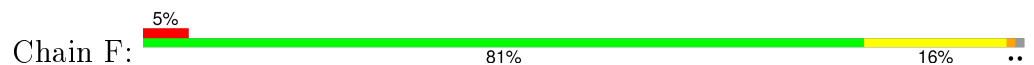
• Molecule 1: Periplasmic oligopeptide-binding protein



• Molecule 1: Periplasmic oligopeptide-binding protein

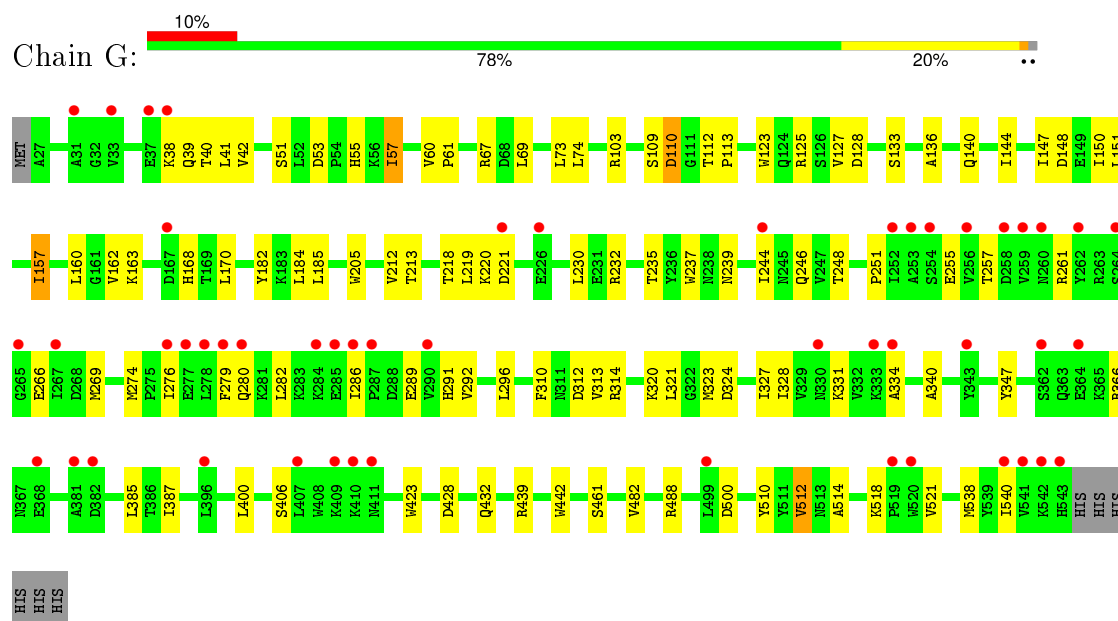


• Molecule 1: Periplasmic oligopeptide-binding protein





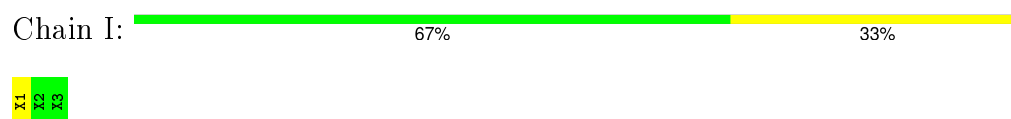
- Molecule 1: Periplasmic oligopeptide-binding protein



- Molecule 1: Periplasmic oligopeptide-binding protein



- Molecule 2: Endogenous peptide



- Molecule 2: Endogenous peptide

Chain J:  67% 33%



- Molecule 2: Endogenous peptide

Chain K:  67% 33%



- Molecule 2: Endogenous peptide

Chain L:  67% 33%



- Molecule 2: Endogenous peptide

Chain M:  33% 67%



- Molecule 2: Endogenous peptide

Chain N:  67% 33%



- Molecule 2: Endogenous peptide

Chain O:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: Endogenous peptide

Chain P:  67% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.62Å 202.60Å 208.95Å 90.00° 95.71° 90.00°	Depositor
Resolution (Å)	48.37 – 2.00 48.37 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.9 (48.37-2.00) 98.9 (48.37-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.6.0104	Depositor
R, R_{free}	0.229 , 0.267 0.230 , 0.267	Depositor DCC
R_{free} test set	17261 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	25.7	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 50.5	EDS
Estimated twinning fraction	0.033 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 345407 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	35615	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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 33.69 % 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 7.6804e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.77	2/4245 (0.0%)	0.80	6/5790 (0.1%)
1	B	0.68	2/4244 (0.0%)	0.71	4/5789 (0.1%)
1	C	0.68	4/4237 (0.1%)	0.68	2/5779 (0.0%)
1	D	0.66	3/4237 (0.1%)	0.69	2/5779 (0.0%)
1	E	0.71	2/4245 (0.0%)	0.74	5/5790 (0.1%)
1	F	0.72	4/4264 (0.1%)	0.71	3/5817 (0.1%)
1	G	0.69	5/4243 (0.1%)	0.70	3/5788 (0.1%)
1	H	0.66	2/4237 (0.0%)	0.64	1/5779 (0.0%)
All	All	0.70	24/33952 (0.1%)	0.71	26/46311 (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	B	0	1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	205	TRP	CD2-CE2	5.75	1.48	1.41
1	A	205	TRP	CD2-CE2	5.72	1.48	1.41
1	F	237	TRP	CD2-CE2	5.70	1.48	1.41
1	G	205	TRP	CD2-CE2	5.63	1.48	1.41
1	D	98	TRP	CD2-CE2	5.58	1.48	1.41
1	E	520	TRP	CD2-CE2	5.51	1.48	1.41
1	F	205	TRP	CD2-CE2	5.46	1.48	1.41
1	H	520	TRP	CD2-CE2	5.34	1.47	1.41
1	A	361	TRP	CD2-CE2	5.32	1.47	1.41
1	C	520	TRP	CD2-CE2	5.29	1.47	1.41
1	F	90	TRP	CD2-CE2	5.29	1.47	1.41
1	E	90	TRP	CD2-CE2	5.28	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	408	TRP	CD2-CE2	5.23	1.47	1.41
1	C	205	TRP	CD2-CE2	5.21	1.47	1.41
1	D	358	TRP	CD2-CE2	5.11	1.47	1.41
1	D	408	TRP	CD2-CE2	5.10	1.47	1.41
1	G	442	TRP	CD2-CE2	5.07	1.47	1.41
1	B	520	TRP	CD2-CE2	5.06	1.47	1.41
1	F	222	TRP	CD2-CE2	5.06	1.47	1.41
1	G	123	TRP	CD2-CE2	5.05	1.47	1.41
1	G	237	TRP	CD2-CE2	5.04	1.47	1.41
1	C	361	TRP	CD2-CE2	5.04	1.47	1.41
1	G	423	TRP	CD2-CE2	5.00	1.47	1.41
1	H	423	TRP	CD2-CE2	5.00	1.47	1.41

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	67	ARG	NE-CZ-NH2	-12.89	113.86	120.30
1	A	67	ARG	NE-CZ-NH2	-10.32	115.14	120.30
1	B	103	ARG	NE-CZ-NH2	-9.74	115.43	120.30
1	A	67	ARG	NE-CZ-NH1	9.53	125.06	120.30
1	B	103	ARG	NE-CZ-NH1	9.42	125.01	120.30
1	D	67	ARG	NE-CZ-NH2	-9.05	115.77	120.30
1	E	67	ARG	NE-CZ-NH1	8.83	124.72	120.30
1	C	67	ARG	NE-CZ-NH2	-8.44	116.08	120.30
1	F	67	ARG	NE-CZ-NH2	-8.13	116.23	120.30
1	F	67	ARG	NE-CZ-NH1	8.11	124.36	120.30
1	D	67	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	C	67	ARG	NE-CZ-NH1	7.81	124.20	120.30
1	F	488	ARG	NE-CZ-NH1	7.63	124.12	120.30
1	B	67	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	G	103	ARG	NE-CZ-NH1	-7.02	116.79	120.30
1	A	488	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	A	488	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	G	103	ARG	NE-CZ-NH2	6.61	123.61	120.30
1	B	67	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	E	232	ARG	NE-CZ-NH2	6.39	123.50	120.30
1	G	67	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	E	232	ARG	NE-CZ-NH1	-6.05	117.28	120.30
1	A	103	ARG	NE-CZ-NH2	5.94	123.27	120.30
1	E	261	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	H	439	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	A	110	ASP	CB-CA-C	-5.19	100.02	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	483	THR	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	4137	0	4046	92	0
1	B	4136	0	4047	59	0
1	C	4129	0	4041	73	0
1	D	4129	0	4041	55	0
1	E	4137	0	4044	69	0
1	F	4155	0	4061	89	0
1	G	4135	0	4046	107	0
1	H	4129	0	4041	99	0
2	I	15	0	5	2	0
2	J	15	0	5	1	0
2	K	15	0	5	1	0
2	L	15	0	5	1	0
2	M	15	0	5	2	0
2	N	15	0	5	1	0
2	O	15	0	5	0	0
2	P	15	0	5	1	0
3	A	360	0	0	35	0
3	B	268	0	0	12	0
3	C	285	0	0	25	0
3	D	265	0	0	9	0
3	E	351	0	0	20	0
3	F	344	0	0	38	0
3	G	305	0	0	33	0
3	H	221	0	0	41	0
3	I	2	0	0	1	0
3	J	2	0	0	0	0
3	K	1	0	0	0	0
3	M	2	0	0	0	0
3	P	2	0	0	1	0
All	All	35615	0	32407	650	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (650) 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:147:ILE:HG21	3:H:3221:HOH:O	1.16	1.33
1:E:158:THR:HG23	3:E:3234:HOH:O	1.21	1.30
1:G:184:LEU:HD22	3:G:3263:HOH:O	1.27	1.29
1:A:457:LEU:HD13	3:A:3253:HOH:O	1.11	1.27
1:F:65:ILE:HG22	3:F:3274:HOH:O	1.26	1.26
1:F:403:ALA:HB3	3:F:2122:HOH:O	1.05	1.23
1:C:193:VAL:CG1	1:C:198:ILE:HD11	1.70	1.21
1:G:185:LEU:HD12	3:G:3189:HOH:O	1.38	1.20
1:A:323:MET:SD	3:A:3197:HOH:O	1.95	1.19
1:C:218:THR:HB	3:C:3250:HOH:O	1.39	1.18
1:C:472:PHE:CE2	3:C:3252:HOH:O	1.97	1.17
1:H:385:LEU:HD12	3:H:3237:HOH:O	1.44	1.16
1:G:269:MET:CE	1:G:538:MET:HE3	1.76	1.15
1:H:185:LEU:HD23	3:H:2390:HOH:O	1.47	1.14
1:G:269:MET:HE1	1:G:538:MET:CE	1.79	1.12
3:E:3220:HOH:O	2:M:3:UNK:C	1.93	1.12
1:G:127:VAL:HG22	3:G:3275:HOH:O	1.49	1.08
1:E:232:ARG:HD3	1:E:239:ASN:HD21	1.18	1.07
1:B:173:THR:HG23	3:B:1116:HOH:O	1.53	1.05
1:C:319:LEU:HD12	3:C:2520:HOH:O	1.56	1.05
1:B:535:THR:HG22	3:B:1831:HOH:O	1.57	1.05
1:A:274:MET:SD	3:A:3172:HOH:O	2.13	1.04
1:A:453:LEU:HB3	1:A:476:MET:HE3	1.38	1.03
1:G:41:LEU:HD21	1:G:269:MET:HE3	1.40	1.03
1:E:206:THR:HG21	3:E:3239:HOH:O	1.62	1.00
1:B:393:THR:HG22	1:B:420:ASN:HD22	1.27	1.00
1:C:193:VAL:HG11	1:C:198:ILE:HD11	1.39	0.98
1:D:220:LYS:NZ	1:D:246:GLN:NE2	2.12	0.98
1:B:323:MET:SD	3:B:3160:HOH:O	2.22	0.97
1:H:456:MET:HE3	1:H:499:LEU:HD11	1.46	0.97
1:F:353:LEU:HD11	3:F:3264:HOH:O	1.62	0.97
1:A:428:ASP:OD2	1:A:432:GLN:NE2	1.98	0.96
1:B:477:ALA:HB1	3:B:3251:HOH:O	1.65	0.96
1:G:269:MET:HE1	1:G:538:MET:HE3	0.96	0.95
1:G:151:LEU:HD21	3:G:3275:HOH:O	1.64	0.95
1:H:242:THR:HG22	3:H:561:HOH:O	1.66	0.94
1:H:160:LEU:HD21	3:H:3244:HOH:O	1.67	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:428:ASP:OD2	1:F:432:GLN:NE2	2.00	0.94
1:D:220:LYS:HZ1	1:D:246:GLN:NE2	1.64	0.94
1:B:386:THR:HG22	1:B:415:ASN:HB2	1.49	0.94
1:E:232:ARG:HD3	1:E:239:ASN:ND2	1.82	0.93
1:A:319:LEU:HD23	3:A:3257:HOH:O	1.68	0.93
1:F:387:ILE:CG2	3:F:3261:HOH:O	2.16	0.93
1:H:456:MET:CE	1:H:499:LEU:HD11	2.00	0.92
1:G:324:ASP:O	1:G:328:ILE:HD12	1.70	0.92
1:C:193:VAL:CG1	1:C:198:ILE:CD1	2.47	0.92
1:G:220:LYS:NZ	1:G:246:GLN:NE2	2.18	0.92
1:D:220:LYS:NZ	1:D:246:GLN:HE21	1.67	0.92
3:A:3286:HOH:O	2:I:1:UNK:CB	2.18	0.90
1:G:220:LYS:HZ1	1:G:246:GLN:HE21	1.16	0.90
1:D:220:LYS:HZ3	1:D:246:GLN:HE21	1.15	0.90
1:E:232:ARG:CD	1:E:239:ASN:HD21	1.84	0.89
1:H:315:VAL:HG21	3:H:3206:HOH:O	1.71	0.89
1:H:538:MET:CE	3:H:3292:HOH:O	2.20	0.89
1:H:160:LEU:CD2	3:H:3244:HOH:O	2.20	0.89
1:C:456:MET:HB2	3:C:3252:HOH:O	1.73	0.89
1:E:428:ASP:OD2	1:E:432:GLN:NE2	2.05	0.88
1:F:387:ILE:HG22	3:F:3261:HOH:O	1.68	0.88
1:E:39:GLN:HE22	1:E:540:ILE:H	1.18	0.88
1:D:540:ILE:HG12	3:D:3217:HOH:O	1.74	0.88
1:F:400:LEU:HD23	3:F:3267:HOH:O	1.74	0.87
1:D:127:VAL:HG13	1:D:151:LEU:CD2	2.05	0.86
1:C:276:ILE:HD12	1:C:399:LYS:HD3	1.58	0.86
1:H:406:SER:HB2	3:H:2605:HOH:O	1.76	0.86
1:C:319:LEU:HB2	3:C:2520:HOH:O	1.75	0.85
2:I:1:UNK:CB	3:I:3280:HOH:O	2.25	0.85
1:D:39:GLN:HE22	1:D:540:ILE:H	1.23	0.85
1:A:282:LEU:HD12	3:A:2233:HOH:O	1.74	0.85
1:G:220:LYS:NZ	1:G:246:GLN:HE21	1.72	0.85
3:C:3176:HOH:O	2:K:1:UNK:CB	2.25	0.85
1:G:274:MET:SD	3:G:3205:HOH:O	2.35	0.85
1:B:380:THR:HG22	3:B:3213:HOH:O	1.77	0.85
1:A:493:THR:HG23	3:A:666:HOH:O	1.77	0.85
1:G:140:GLN:HG3	1:G:147:ILE:HD13	1.59	0.84
1:G:40:THR:O	1:G:540:ILE:HD11	1.77	0.84
1:D:143:HIS:CD2	1:D:480:LEU:HD11	2.11	0.84
1:F:344:THR:HG22	3:F:3264:HOH:O	1.76	0.84
1:A:39:GLN:HE22	1:A:540:ILE:H	1.23	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:269:MET:CE	1:G:538:MET:CE	2.47	0.83
1:G:220:LYS:HZ2	1:G:246:GLN:NE2	1.77	0.83
1:G:182:TYR:HA	3:G:3189:HOH:O	1.78	0.82
1:G:57:ILE:HG23	3:G:2129:HOH:O	1.79	0.82
1:G:39:GLN:HE22	1:G:540:ILE:H	1.26	0.81
1:H:213:THR:OG1	1:H:218:THR:HG22	1.80	0.81
1:F:535[A]:THR:HG22	3:F:1234:HOH:O	1.80	0.81
1:E:493:THR:HG23	3:E:949:HOH:O	1.81	0.81
1:H:140:GLN:HA	3:H:3221:HOH:O	1.81	0.80
1:F:213:THR:OG1	1:F:218:THR:HG22	1.82	0.80
1:C:317:THR:HG22	1:C:503:SER:OG	1.82	0.79
1:A:476:MET:CE	1:A:495:ALA:HB1	2.12	0.79
1:C:39:GLN:HA	1:C:540:ILE:HD13	1.62	0.79
1:A:476:MET:HE2	1:A:495:ALA:HB1	1.62	0.79
1:C:193:VAL:HG12	1:C:198:ILE:CD1	2.13	0.79
1:A:453:LEU:HD13	1:A:476:MET:HE1	1.65	0.78
1:C:456:MET:C	3:C:3252:HOH:O	2.22	0.78
1:F:220:LYS:HZ3	1:F:246:GLN:HE21	1.29	0.78
1:G:53:ASP:O	1:G:57:ILE:HD13	1.84	0.78
1:E:53:ASP:N	3:E:3239:HOH:O	2.16	0.77
1:H:482:VAL:HG22	1:H:487:GLN:NE2	1.99	0.77
1:F:65:ILE:CG2	3:F:3274:HOH:O	2.01	0.77
1:C:193:VAL:HG13	1:C:194:PRO:HD2	1.66	0.77
1:C:456:MET:CB	3:C:3252:HOH:O	2.32	0.77
1:A:483:THR:HG22	1:A:484:ASP:OD1	1.85	0.77
1:A:237:TRP:CZ2	3:A:3207:HOH:O	2.35	0.76
1:G:69:LEU:HD21	1:G:230:LEU:HD22	1.66	0.76
1:B:34:THR:HG23	3:B:2193:HOH:O	1.85	0.76
1:G:296:LEU:HD23	1:G:347:TYR:CE2	2.20	0.75
3:E:2276:HOH:O	2:M:1:UNK:CB	2.32	0.75
1:H:185:LEU:HA	3:H:2390:HOH:O	1.86	0.74
1:C:482:VAL:HG12	1:C:484:ASP:H	1.52	0.74
1:D:40:THR:O	1:D:540:ILE:HD11	1.87	0.73
1:C:176:GLU:HG2	1:C:480:LEU:HB3	1.71	0.73
1:D:274:MET:SD	3:D:3195:HOH:O	2.46	0.73
1:G:286:ILE:HG21	1:G:289:GLU:CD	2.08	0.73
1:F:480:LEU:HD23	1:F:488:ARG:HH21	1.54	0.73
1:C:316:ARG:HA	3:C:2520:HOH:O	1.89	0.72
1:F:127:VAL:HG12	1:F:150:ILE:HG22	1.70	0.72
1:H:49:VAL:HG22	3:H:2458:HOH:O	1.89	0.72
1:E:128:ASP:HA	1:E:157:ILE:HD11	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:150:ILE:HG23	1:H:157:ILE:HD12	1.72	0.72
1:F:385:LEU:HG	1:F:387:ILE:HD13	1.72	0.72
1:A:476:MET:CE	1:A:495:ALA:CB	2.68	0.71
1:A:53:ASP:HA	3:A:3229:HOH:O	1.90	0.71
1:G:127:VAL:HG12	1:G:150:ILE:HG22	1.72	0.71
1:D:274:MET:HE2	1:D:279:PHE:CD2	2.26	0.70
1:A:476:MET:HE1	1:A:495:ALA:CB	2.21	0.70
1:B:286:ILE:HG22	1:B:286:ILE:O	1.90	0.70
1:C:218:THR:CB	3:C:3250:HOH:O	2.13	0.70
1:H:190:THR:HG21	3:H:2390:HOH:O	1.90	0.70
1:H:232:ARG:HE	1:H:239:ASN:HD21	1.38	0.70
1:B:248:THR:HG23	3:B:828:HOH:O	1.91	0.70
1:E:428:ASP:OD1	1:E:432:GLN:NE2	2.23	0.70
1:F:69:LEU:HG	3:F:3274:HOH:O	1.90	0.70
1:A:205:TRP:CH2	3:A:3229:HOH:O	2.44	0.70
1:F:453:LEU:HB2	3:F:3223:HOH:O	1.90	0.70
1:A:261:ARG:HD3	1:A:266:GLU:OE2	1.92	0.70
1:G:127:VAL:HG13	3:G:3275:HOH:O	1.92	0.70
1:F:416:VAL:HG13	3:F:3261:HOH:O	1.92	0.70
1:A:205:TRP:CZ2	3:A:3229:HOH:O	2.44	0.69
1:E:428:ASP:CG	1:E:432:GLN:NE2	2.46	0.69
1:F:286:ILE:O	1:F:286:ILE:HG22	1.90	0.69
1:E:157:ILE:HG22	3:E:3234:HOH:O	1.92	0.69
1:G:257:THR:HG21	3:G:1413:HOH:O	1.92	0.69
1:G:136:ALA:HB3	3:G:2204:HOH:O	1.93	0.69
1:F:344:THR:CG2	3:F:3264:HOH:O	2.36	0.69
1:B:456:MET:CE	1:B:499:LEU:HD11	2.23	0.69
1:F:39:GLN:HE22	1:F:540:ILE:H	1.38	0.69
1:B:323:MET:HE1	1:B:328:ILE:CD1	2.23	0.69
1:F:493[A]:THR:HG23	3:F:1094:HOH:O	1.91	0.69
1:G:162:VAL:HG12	1:G:170:LEU:HD11	1.74	0.68
1:H:52:LEU:HD12	1:H:222:TRP:CZ3	2.29	0.68
1:G:41:LEU:CD2	1:G:269:MET:HE3	2.22	0.68
1:D:274:MET:HE2	1:D:279:PHE:HD2	1.59	0.68
1:H:538:MET:HE2	3:H:3292:HOH:O	1.83	0.68
1:E:456:MET:HE2	1:E:499:LEU:HD11	1.76	0.67
1:A:310:PHE:HE1	3:A:3257:HOH:O	1.77	0.67
1:C:317:THR:OG1	1:C:373:LEU:HD13	1.94	0.67
1:H:236:TYR:CZ	3:H:3291:HOH:O	2.47	0.67
1:E:428:ASP:CG	1:E:432:GLN:HE21	1.98	0.67
1:D:127:VAL:HG13	1:D:151:LEU:HD21	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:218:THR:HG21	3:D:2464:HOH:O	1.93	0.67
1:B:296:LEU:HD22	1:B:348[A]:THR:HG22	1.77	0.67
1:H:73:LEU:HD12	1:H:185:LEU:HD13	1.76	0.67
1:H:352:LYS:O	1:H:493:THR:HG21	1.95	0.67
1:C:493:THR:HG23	3:C:2120:HOH:O	1.93	0.67
1:B:456:MET:HE3	1:B:499:LEU:HD11	1.75	0.66
1:A:39:GLN:HE22	1:A:540:ILE:N	1.92	0.66
1:F:335:GLN:NE2	3:F:3260:HOH:O	2.28	0.66
1:H:127:VAL:HG13	1:H:151:LEU:CD2	2.26	0.66
1:F:386:THR:HG22	1:F:415:ASN:HD22	1.60	0.66
1:A:312:ASP:OD2	1:A:314:ARG:HD3	1.95	0.66
1:A:110:ASP:HB3	1:A:112:THR:HG23	1.78	0.66
1:G:428:ASP:OD2	1:G:432:GLN:NE2	2.29	0.66
1:F:220:LYS:NZ	1:F:246:GLN:HE21	1.94	0.66
1:C:349:ASP:HB3	3:C:3228:HOH:O	1.95	0.66
1:G:518:LYS:HB2	3:G:3259:HOH:O	1.96	0.65
1:B:220:LYS:HD2	3:B:3283:HOH:O	1.95	0.65
1:E:39:GLN:HA	1:E:540:ILE:HD13	1.77	0.65
1:F:127:VAL:CG1	1:F:150:ILE:HG22	2.25	0.65
1:B:393:THR:CG2	1:B:420:ASN:HD22	2.06	0.65
1:E:165:ILE:HD11	1:E:171:GLU:HB2	1.78	0.65
1:H:309:PRO:HB2	3:H:3206:HOH:O	1.96	0.65
1:H:48:GLU:HG2	3:H:2455:HOH:O	1.97	0.65
1:F:386:THR:HG22	1:F:415:ASN:HB2	1.78	0.65
1:D:92:ASN:HD22	1:D:95:ALA:H	1.45	0.64
1:A:123:TRP:O	1:A:126[B]:SER:OG	2.16	0.64
1:H:69:LEU:HD21	1:H:230:LEU:HD22	1.79	0.64
1:D:173:THR:HG23	3:D:1678:HOH:O	1.98	0.64
1:G:128:ASP:HA	1:G:157:ILE:HD11	1.78	0.64
1:A:480:LEU:HD23	1:A:488:ARG:HH21	1.62	0.64
1:A:165:ILE:HD11	1:A:171:GLU:HB2	1.80	0.64
1:B:386:THR:HG22	1:B:415:ASN:HD22	1.63	0.63
1:H:39:GLN:HE22	1:H:540:ILE:H	1.46	0.63
1:H:147:ILE:HD13	3:H:3221:HOH:O	1.97	0.63
1:E:456:MET:CE	1:E:499:LEU:HD11	2.29	0.63
1:E:124:GLN:HB3	1:E:157:ILE:HG23	1.80	0.63
1:G:185:LEU:CD1	3:G:3189:HOH:O	2.17	0.63
1:F:220:LYS:NZ	1:F:246:GLN:NE2	2.47	0.63
1:A:296:LEU:HD23	1:A:347:TYR:CE2	2.34	0.63
1:D:310:PHE:HZ	1:D:387:ILE:HG21	1.63	0.62
3:A:1774:HOH:O	1:C:313:VAL:HG23	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:LEU:CD1	3:A:2233:HOH:O	2.38	0.62
1:E:488:ARG:NH2	3:E:2202:HOH:O	2.27	0.62
1:F:220:LYS:NZ	3:F:2779:HOH:O	2.32	0.62
3:B:2264:HOH:O	2:J:1:UNK:CB	2.48	0.62
1:G:144:ILE:O	1:G:147:ILE:HG13	1.99	0.62
1:D:220:LYS:HZ1	1:D:246:GLN:HE22	1.42	0.62
1:F:480:LEU:HD23	1:F:488:ARG:NH2	2.15	0.62
1:C:218:THR:HG23	1:C:233:SER:HB2	1.81	0.62
1:D:45:ASN:ND2	1:D:64:ASN:HD22	1.97	0.61
1:E:269:MET:CG	3:E:1154:HOH:O	2.47	0.61
1:C:71:GLU:O	1:C:214:ASN:ND2	2.33	0.61
1:F:410:LYS:HD2	3:F:3294:HOH:O	2.00	0.61
1:H:128:ASP:HA	1:H:157:ILE:HD11	1.81	0.61
1:G:324:ASP:O	1:G:328:ILE:CD1	2.45	0.61
3:F:3269:HOH:O	2:N:1:UNK:CB	2.47	0.61
1:H:143:HIS:NE2	3:H:3262:HOH:O	2.23	0.61
1:E:269:MET:SD	3:E:1154:HOH:O	2.56	0.61
1:F:220:LYS:HZ3	1:F:246:GLN:NE2	1.98	0.61
1:C:193:VAL:HG11	1:C:198:ILE:CD1	2.22	0.60
1:G:41:LEU:HD11	1:G:269:MET:HE2	1.84	0.60
1:C:310:PHE:HZ	1:C:387:ILE:HG21	1.66	0.60
1:G:220:LYS:HZ2	1:G:246:GLN:HE22	1.49	0.60
1:A:54:PRO:HD3	3:A:3229:HOH:O	2.00	0.60
1:H:39:GLN:NE2	1:H:243:VAL:HG12	2.16	0.60
1:E:124:GLN:HB3	1:E:157:ILE:CG2	2.31	0.60
1:H:480:LEU:HD11	3:H:3262:HOH:O	2.01	0.60
1:A:385:LEU:HG	1:A:387:ILE:HD13	1.83	0.60
1:H:127:VAL:HG12	1:H:150:ILE:HG22	1.83	0.60
1:C:313:VAL:O	1:C:317:THR:HG23	2.01	0.60
1:A:345:PRO:O	1:A:348:THR:CG2	2.49	0.60
1:A:319:LEU:CD2	3:A:3257:HOH:O	2.38	0.60
1:H:220:LYS:HZ1	1:H:246:GLN:NE2	1.99	0.60
1:D:71:GLU:O	1:D:214:ASN:ND2	2.35	0.60
1:A:499:LEU:HG	3:A:3293:HOH:O	1.99	0.60
1:F:128:ASP:HA	1:F:157:ILE:HD11	1.84	0.60
1:C:286:ILE:O	1:C:286:ILE:HD12	2.03	0.59
1:E:352:LYS:O	1:E:493:THR:HG21	2.03	0.59
1:C:310:PHE:CD2	3:C:2179:HOH:O	2.52	0.59
1:G:147:ILE:HD11	3:G:599:HOH:O	2.02	0.59
1:H:232:ARG:HE	1:H:239:ASN:ND2	2.02	0.58
1:H:309:PRO:CG	3:H:3206:HOH:O	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:456:MET:HE3	1:E:467:TYR:CD1	2.39	0.58
1:B:262:TYR:CZ	1:B:518:LYS:HD3	2.39	0.58
1:C:193:VAL:HG12	1:C:198:ILE:HD12	1.83	0.58
1:A:345:PRO:O	1:A:348:THR:HG23	2.03	0.58
1:A:232:ARG:HE	1:A:239:ASN:HD21	1.52	0.58
1:F:476:MET:CE	3:F:3223:HOH:O	2.52	0.58
1:A:344:THR:HG23	1:A:496:GLU:OE2	2.04	0.58
1:G:269:MET:HE2	1:G:521:VAL:HG11	1.86	0.58
1:F:514:ALA:HB3	3:F:3186:HOH:O	2.04	0.58
1:A:453:LEU:HB3	1:A:476:MET:CE	2.26	0.57
1:B:380:THR:HA	3:B:3213:HOH:O	2.04	0.57
1:A:256:VAL:HG23	1:A:395:ASP:OD2	2.04	0.57
1:C:482:VAL:CG1	1:C:487:GLN:HB2	2.34	0.57
1:H:274:MET:HE1	1:H:282:LEU:HD13	1.85	0.57
1:C:310:PHE:HE1	1:C:319:LEU:HD11	1.69	0.57
1:A:217:TYR:OH	1:A:535:THR:HG22	2.04	0.57
1:H:99:THR:HG23	3:H:1470:HOH:O	2.04	0.57
1:D:274:MET:CE	1:D:279:PHE:HD2	2.17	0.57
1:G:113:PRO:HG2	3:G:2745:HOH:O	2.05	0.57
2:P:3:UNK:C	3:P:455:HOH:O	2.52	0.57
1:G:312:ASP:OD2	1:G:314:ARG:HD3	2.04	0.57
1:B:323:MET:HE1	1:B:328:ILE:HG12	1.86	0.57
1:G:147:ILE:HG23	1:G:160:LEU:HD11	1.86	0.57
1:H:127:VAL:HG13	1:H:151:LEU:HD23	1.87	0.56
1:G:323:MET:SD	1:G:328:ILE:HD11	2.45	0.56
1:F:286:ILE:HG22	1:F:289:GLU:HB2	1.86	0.56
1:H:220:LYS:NZ	1:H:246:GLN:NE2	2.53	0.56
1:B:363:GLN:NE2	1:B:366:ARG:NH2	2.53	0.56
1:D:353:LEU:HA	1:D:493:THR:CG2	2.36	0.56
1:D:312:ASP:OD2	1:D:314:ARG:HD3	2.06	0.56
1:H:456:MET:HE2	1:H:499:LEU:HD11	1.84	0.56
1:C:317:THR:HG22	1:C:503:SER:HG	1.71	0.56
1:H:456:MET:HE3	1:H:499:LEU:CD1	2.30	0.56
1:F:330:ASN:O	1:F:333:LYS:NZ	2.39	0.56
1:G:232:ARG:HE	1:G:239:ASN:HD21	1.52	0.56
1:G:279:PHE:N	3:G:3231:HOH:O	2.38	0.56
1:E:261:ARG:HD3	1:E:266:GLU:OE2	2.05	0.56
1:B:123:TRP:HE3	1:B:162:VAL:HG21	1.71	0.56
1:C:296:LEU:HD23	1:C:347:TYR:CE1	2.40	0.56
1:F:385:LEU:HG	1:F:387:ILE:CD1	2.34	0.55
1:A:345:PRO:HB2	1:A:348:THR:HG22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:HIS:NE2	1:D:480:LEU:HD11	2.21	0.55
1:H:216:ALA:HB2	3:H:3291:HOH:O	2.06	0.55
1:F:491:LEU:HD23	3:F:1702:HOH:O	2.07	0.55
1:B:491:LEU:HD23	1:B:494:LYS:HE3	1.89	0.55
1:H:129:PRO:HD3	3:H:2123:HOH:O	2.06	0.55
1:A:55:HIS:HE1	3:A:736:HOH:O	1.90	0.55
1:B:363:GLN:NE2	1:B:366:ARG:HH21	2.05	0.54
1:C:240:ALA:HB3	3:C:2465:HOH:O	2.05	0.54
1:G:269:MET:CE	1:G:521:VAL:HG11	2.38	0.54
1:D:127:VAL:HG13	1:D:151:LEU:HD23	1.89	0.54
1:D:37:GLU:HB3	3:D:2127:HOH:O	2.07	0.54
1:F:320:LYS:HA	1:F:506:VAL:HG13	1.90	0.54
1:A:363:GLN:NE2	1:A:366:ARG:HE	2.06	0.54
1:D:232:ARG:HE	1:D:239:ASN:HD21	1.54	0.54
1:B:323:MET:CE	1:B:328:ILE:HD13	2.38	0.54
1:D:45:ASN:HD21	1:D:64:ASN:HD22	1.56	0.54
1:G:296:LEU:HD23	1:G:347:TYR:CD2	2.43	0.53
1:A:324:ASP:OD2	1:A:327:ILE:HD12	2.07	0.53
1:B:286:ILE:HG22	1:B:289:GLU:HB2	1.91	0.53
1:A:55:HIS:CD2	1:A:125:ARG:HH11	2.27	0.53
1:E:55:HIS:HE1	3:E:1549:HOH:O	1.90	0.53
1:H:143:HIS:NE2	1:H:480:LEU:HD11	2.23	0.53
1:G:127:VAL:HG12	1:G:150:ILE:CG2	2.39	0.53
1:E:55:HIS:CD2	1:E:125:ARG:HH11	2.26	0.53
1:H:27:ALA:N	1:H:241:LYS:O	2.41	0.53
1:A:498:GLN:NE2	3:A:3152:HOH:O	2.40	0.53
1:A:276:ILE:HG23	1:A:331:LYS:O	2.08	0.53
1:B:55:HIS:HE1	3:B:1032:HOH:O	1.90	0.53
1:A:407:LEU:HD13	3:A:3197:HOH:O	2.08	0.53
1:C:349:ASP:CB	3:C:3228:HOH:O	2.54	0.53
1:C:73:LEU:C	1:C:74:LEU:HD23	2.29	0.53
1:A:407:LEU:CD1	3:A:3197:HOH:O	2.56	0.53
1:E:353:LEU:HD23	1:E:493:THR:HG22	1.91	0.53
1:A:270:THR:HG23	1:A:516:LEU:HB2	1.91	0.53
1:D:482:VAL:CG1	1:D:484:ASP:O	2.57	0.53
1:A:389:LEU:HD22	3:A:3282:HOH:O	2.09	0.53
1:H:309:PRO:CB	3:H:3206:HOH:O	2.55	0.52
1:B:386:THR:HG22	1:B:415:ASN:CB	2.33	0.52
1:E:130:ASN:HB3	3:E:2203:HOH:O	2.10	0.52
1:A:319:LEU:CG	3:A:3257:HOH:O	2.56	0.52
1:H:220:LYS:NZ	1:H:246:GLN:HE21	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:LEU:CG	3:A:3293:HOH:O	2.56	0.52
1:G:310:PHE:HZ	1:G:387:ILE:CG1	2.23	0.52
1:C:218:THR:CG2	1:C:233:SER:HB2	2.40	0.52
1:F:217:TYR:CE2	1:F:535[A]:THR:OG1	2.61	0.52
1:H:364:GLU:H	1:H:364:GLU:CD	2.13	0.52
1:H:363:GLN:HE21	1:H:366:ARG:HH21	1.57	0.52
1:D:162:VAL:HG13	1:D:172:VAL:HG22	1.92	0.52
1:G:328:ILE:HG23	1:G:400:LEU:HD22	1.91	0.52
1:H:479:THR:HA	3:H:3242:HOH:O	2.10	0.52
1:G:162:VAL:CG1	1:G:170:LEU:HD11	2.38	0.52
1:A:165:ILE:HD11	1:A:171:GLU:CB	2.39	0.52
1:F:389:LEU:HB2	3:F:3261:HOH:O	2.10	0.52
1:C:349:ASP:O	1:C:449:PRO:HD3	2.10	0.52
1:H:491:LEU:HD12	3:H:3242:HOH:O	2.10	0.51
1:F:324:ASP:O	1:F:328:ILE:HD13	2.09	0.51
1:B:399:LYS:NZ	3:B:2260:HOH:O	2.43	0.51
1:F:69:LEU:CD1	3:F:3274:HOH:O	2.59	0.51
1:H:218:THR:HG23	1:H:233:SER:HB2	1.92	0.51
1:A:276:ILE:HD11	1:A:396:LEU:CD1	2.40	0.51
1:G:218:THR:HG22	1:G:219:LEU:H	1.75	0.51
1:C:350:GLY:O	1:C:489:THR:HG22	2.11	0.51
1:H:340:ALA:HA	1:H:510:TYR:CE2	2.45	0.51
1:E:363:GLN:NE2	1:E:366:ARG:HE	2.09	0.51
1:H:319:LEU:HD12	1:H:408:TRP:CE2	2.45	0.51
1:B:386:THR:CG2	1:B:415:ASN:HD22	2.24	0.51
1:G:127:VAL:HG13	1:G:151:LEU:CD2	2.40	0.51
1:A:387:ILE:HG22	1:A:416:VAL:HG13	1.92	0.51
1:F:127:VAL:HG12	1:F:150:ILE:CG2	2.39	0.51
1:C:482:VAL:HG13	1:C:487:GLN:HB2	1.93	0.51
1:F:476:MET:HE2	3:F:3223:HOH:O	2.10	0.51
1:B:55:HIS:CD2	1:B:125:ARG:HH11	2.28	0.51
1:A:384:PRO:HA	3:A:2492:HOH:O	2.09	0.51
1:F:127:VAL:CG1	1:F:127:VAL:O	2.58	0.50
1:G:310:PHE:HZ	1:G:387:ILE:HG13	1.76	0.50
1:C:310:PHE:CE2	3:C:2179:HOH:O	2.64	0.50
1:E:52:LEU:C	3:E:3239:HOH:O	2.48	0.50
1:D:213:THR:OG1	1:D:218:THR:HG23	2.11	0.50
1:E:292:VAL:HG13	1:E:512:VAL:CG1	2.41	0.50
1:G:244:ILE:HD12	1:G:538:MET:HB2	1.94	0.50
1:G:521:VAL:CG2	3:G:3259:HOH:O	2.60	0.50
1:E:55:HIS:HD2	1:E:125:ARG:HH11	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:482:VAL:HG21	3:H:3242:HOH:O	2.11	0.50
1:C:218:THR:HG21	3:C:1599:HOH:O	2.12	0.50
1:D:38:LYS:O	1:D:540:ILE:HD12	2.11	0.50
1:G:128:ASP:CA	1:G:157:ILE:HD11	2.42	0.50
1:G:55:HIS:CD2	1:G:125:ARG:HH11	2.30	0.50
1:D:55:HIS:CD2	1:D:125:ARG:HH11	2.30	0.50
1:E:207:GLN:HG3	1:E:208:PRO:HD2	1.93	0.50
1:E:261:ARG:CD	1:E:266:GLU:OE2	2.60	0.49
1:H:220:LYS:HZ3	1:H:231:GLU:HG2	1.77	0.49
1:B:323:MET:HE1	1:B:328:ILE:CG1	2.42	0.49
1:H:224:VAL:HG13	3:H:2455:HOH:O	2.12	0.49
1:E:162:VAL:HG12	1:E:170:LEU:HD11	1.95	0.49
1:H:242:THR:HG21	3:H:1088:HOH:O	2.11	0.49
1:H:72:GLY:O	1:H:86:VAL:HG23	2.13	0.49
1:D:232:ARG:HE	1:D:239:ASN:ND2	2.10	0.49
1:A:69:LEU:O	1:A:213:THR:HB	2.13	0.49
1:F:55:HIS:HE1	3:F:1079:HOH:O	1.94	0.49
1:F:283:LYS:HA	1:F:290:VAL:HG21	1.95	0.49
1:E:67:ARG:NH2	3:E:827:HOH:O	2.45	0.49
1:G:324:ASP:OD2	1:G:327:ILE:HD12	2.12	0.49
1:D:274:MET:HE1	1:D:282:LEU:HD13	1.94	0.49
1:C:55:HIS:CD2	1:C:125:ARG:HH11	2.29	0.49
1:C:59:GLY:HA3	1:C:62:GLU:OE1	2.13	0.49
1:C:482:VAL:HG11	1:C:484:ASP:O	2.13	0.49
1:C:114:VAL:HG21	1:C:214:ASN:OD1	2.13	0.49
1:C:307:LYS:NZ	3:C:1868:HOH:O	2.38	0.49
1:G:280:GLN:HE21	1:G:334:ALA:HB2	1.78	0.49
1:A:476:MET:HE2	1:A:495:ALA:CB	2.34	0.48
1:F:400:LEU:HA	3:F:3267:HOH:O	2.12	0.48
1:B:345:PRO:HB2	1:B:348[A]:THR:HG23	1.95	0.48
3:E:3240:HOH:O	1:F:37:GLU:HG2	2.13	0.48
1:C:244:ILE:CD1	1:C:539:TYR:HA	2.43	0.48
1:G:127:VAL:CG2	3:G:3275:HOH:O	2.29	0.48
1:H:73:LEU:CD1	1:H:185:LEU:HD13	2.43	0.48
1:D:261:ARG:HD2	1:D:266:GLU:OE2	2.13	0.48
1:C:310:PHE:CE1	1:C:319:LEU:HD11	2.47	0.48
1:G:53:ASP:O	1:G:57:ILE:CD1	2.59	0.48
1:G:244:ILE:CD1	1:G:538:MET:HB2	2.44	0.48
1:B:323:MET:CE	1:B:328:ILE:CD1	2.91	0.48
1:B:300:TYR:CE1	1:B:505:ILE:HD12	2.49	0.48
1:C:220:LYS:HB2	1:C:231:GLU:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:124:GLN:HB3	1:H:157:ILE:HG23	1.95	0.48
1:H:482:VAL:HG13	1:H:483:THR:N	2.28	0.48
1:B:69:LEU:O	1:B:213:THR:HB	2.14	0.48
1:G:274:MET:HE2	1:G:279:PHE:HD2	1.78	0.48
1:G:232:ARG:HE	1:G:239:ASN:ND2	2.12	0.48
1:A:521:VAL:CG1	1:A:538:MET:CE	2.92	0.48
1:E:39:GLN:NE2	1:E:540:ILE:HD12	2.29	0.47
1:G:69:LEU:O	1:G:213:THR:HB	2.14	0.47
1:E:383:LYS:CE	3:G:2188:HOH:O	2.61	0.47
1:H:363:GLN:NE2	1:H:366:ARG:HH21	2.12	0.47
1:F:242:THR:HG21	3:F:858:HOH:O	2.12	0.47
1:H:482:VAL:CG2	3:H:3242:HOH:O	2.62	0.47
1:A:296:LEU:HD23	1:A:347:TYR:CD2	2.49	0.47
1:C:491:LEU:HD23	1:C:494:LYS:HD2	1.96	0.47
1:A:269:MET:HG2	1:A:517:VAL:HG13	1.96	0.47
1:E:124:GLN:CB	1:E:157:ILE:HG23	2.42	0.47
1:E:292:VAL:HG13	1:E:512:VAL:HG13	1.95	0.47
1:A:353:LEU:HA	1:A:493:THR:HG22	1.96	0.47
1:H:92:ASN:HD22	1:H:95:ALA:H	1.62	0.47
1:B:340:ALA:HA	1:B:510:TYR:CE2	2.50	0.47
1:G:73:LEU:C	1:G:74:LEU:HD23	2.34	0.47
1:D:127:VAL:HG12	1:D:127:VAL:O	2.15	0.47
1:E:383:LYS:HE2	3:G:2188:HOH:O	2.13	0.47
1:G:41:LEU:HD11	1:G:269:MET:CE	2.45	0.47
1:B:323:MET:CE	1:B:328:ILE:HG12	2.44	0.47
1:E:409:LYS:HB2	3:E:2517:HOH:O	2.14	0.47
1:C:49:VAL:HG22	3:C:3216:HOH:O	2.15	0.47
1:G:73:LEU:O	1:G:74:LEU:HD23	2.15	0.47
1:H:45:ASN:ND2	1:H:64:ASN:HD22	2.13	0.47
1:F:525:THR:O	1:F:527:LYS:NZ	2.38	0.46
1:A:448:GLU:CD	1:A:449:PRO:HD2	2.35	0.46
1:E:277:GLU:HG3	1:E:399:LYS:HZ1	1.80	0.46
1:H:165:ILE:N	1:H:165:ILE:HD12	2.31	0.46
1:F:91:ASP:C	3:F:3255:HOH:O	2.52	0.46
1:A:217:TYR:CZ	1:A:535:THR:HG22	2.51	0.46
1:D:55:HIS:HD2	1:D:125:ARG:HH11	1.63	0.46
1:E:399:LYS:NZ	3:E:2097:HOH:O	2.35	0.46
1:B:485:GLU:OE2	1:B:488:ARG:NH1	2.49	0.46
1:H:482:VAL:HG21	1:H:487:GLN:HB3	1.97	0.46
1:H:39:GLN:HA	1:H:540:ILE:HD13	1.98	0.46
1:A:405:SER:N	3:A:3282:HOH:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ILE:H	1:A:165:ILE:HD12	1.81	0.46
1:G:127:VAL:CG1	3:G:3275:HOH:O	2.60	0.46
1:D:117:GLN:HG3	3:D:2160:HOH:O	2.16	0.46
1:F:123:TRP:HE3	1:F:162:VAL:HG21	1.81	0.46
1:E:52:LEU:HD13	1:E:219:LEU:HD22	1.98	0.46
1:A:207:GLN:HG3	1:A:208:PRO:HD2	1.98	0.46
1:E:330:ASN:HB3	3:E:3278:HOH:O	2.15	0.46
1:C:310:PHE:HE1	1:C:319:LEU:CD1	2.28	0.46
1:H:171:GLU:HB3	3:H:2194:HOH:O	2.15	0.46
1:G:428:ASP:HB2	3:G:2431:HOH:O	2.14	0.46
1:E:165:ILE:CD1	1:E:171:GLU:HB2	2.44	0.46
1:E:363:GLN:HE21	1:E:366:ARG:HH21	1.64	0.46
1:B:323:MET:HE3	1:B:328:ILE:HD13	1.98	0.45
1:G:55:HIS:HE1	3:G:2761:HOH:O	1.99	0.45
1:E:141:TYR:CE2	1:E:454:ASN:HB3	2.51	0.45
1:G:276:ILE:HG23	1:G:331:LYS:O	2.17	0.45
1:F:286:ILE:CG2	1:F:289:GLU:CD	2.84	0.45
1:D:482:VAL:HG22	1:D:487:GLN:HB3	1.97	0.45
1:A:114:VAL:HG21	1:A:214[A]:ASN:OD1	2.16	0.45
1:E:482:VAL:CG1	1:E:484:ASP:O	2.64	0.45
1:D:319:LEU:HD12	1:D:408:TRP:CE2	2.51	0.45
1:B:49:VAL:HG11	1:B:65:ILE:HD12	1.98	0.45
1:A:352:LYS:O	1:A:493:THR:HG21	2.17	0.45
1:D:482:VAL:HG11	1:D:484:ASP:O	2.16	0.45
1:C:456:MET:CA	3:C:3252:HOH:O	2.59	0.45
1:F:45:ASN:ND2	1:F:64:ASN:HD22	2.13	0.45
1:F:232:ARG:HE	1:F:239:ASN:HD21	1.65	0.45
1:A:67:ARG:NH2	3:A:3030:HOH:O	2.49	0.45
1:F:340:ALA:HA	1:F:510:TYR:CE2	2.52	0.45
1:F:428:ASP:CG	1:F:432:GLN:HE21	2.19	0.45
1:G:220:LYS:HZ1	1:G:246:GLN:NE2	1.87	0.45
1:A:385:LEU:HG	1:A:387:ILE:CD1	2.46	0.45
1:B:444:ALA:HB3	1:B:530:LEU:CD2	2.47	0.45
1:C:193:VAL:HG13	1:C:198:ILE:HD11	1.86	0.45
1:G:147:ILE:HD12	1:G:148:ASP:N	2.32	0.45
1:G:261:ARG:HD3	1:G:266:GLU:OE2	2.16	0.45
1:G:320:LYS:NZ	1:G:500:ASP:O	2.50	0.45
1:F:127:VAL:CG1	1:F:150:ILE:CG2	2.92	0.45
1:D:409:LYS:HZ3	1:D:415:ASN:HA	1.82	0.45
1:H:172:VAL:HG11	1:H:181:PHE:CZ	2.51	0.45
1:C:141:TYR:CE1	1:C:454:ASN:HB3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:212:VAL:HG11	3:G:2550:HOH:O	2.18	0.45
1:F:310:PHE:HZ	1:F:387:ILE:CG1	2.29	0.44
1:A:422:GLU:HG2	3:A:2751:HOH:O	2.17	0.44
1:G:540:ILE:HG12	3:G:3201:HOH:O	2.16	0.44
1:B:229:VAL:HG22	1:B:248:THR:HG22	1.99	0.44
1:G:385:LEU:HG	1:G:387:ILE:CD1	2.47	0.44
1:D:59:GLY:HA3	1:D:62:GLU:OE2	2.17	0.44
1:C:50:GLN:HA	1:C:424:LYS:HD3	1.99	0.44
1:F:27:ALA:HB3	1:F:243:VAL:HG23	1.99	0.44
1:G:292:VAL:HG13	1:G:512:VAL:CG1	2.46	0.44
1:F:476:MET:HE1	3:F:3223:HOH:O	2.17	0.44
1:D:310:PHE:HZ	1:D:387:ILE:CG2	2.29	0.44
1:B:166:ASP:HB3	1:B:168:HIS:H	1.82	0.44
1:D:350:GLY:O	1:D:489:THR:HG23	2.18	0.44
1:F:127:VAL:HG12	1:F:127:VAL:O	2.17	0.44
1:F:453:LEU:CB	3:F:3223:HOH:O	2.57	0.44
1:H:352:LYS:O	1:H:493:THR:CG2	2.65	0.44
1:G:110:ASP:HB3	1:G:112:THR:HG23	2.00	0.44
1:H:81:HIS:HD2	3:H:2341:HOH:O	2.01	0.44
1:H:39:GLN:NE2	1:H:540:ILE:HD12	2.33	0.44
1:H:349:ASP:O	1:H:449:PRO:HD3	2.17	0.44
1:E:103:ARG:HD3	1:E:237:TRP:CD2	2.52	0.44
1:H:123:TRP:HB3	3:H:3244:HOH:O	2.18	0.44
1:D:69:LEU:O	1:D:213:THR:HB	2.18	0.44
1:G:109:SER:HA	1:G:235:THR:OG1	2.17	0.44
1:F:69:LEU:CG	3:F:3274:HOH:O	2.58	0.44
1:G:218:THR:HG22	1:G:219:LEU:N	2.32	0.44
1:G:321:LEU:HD22	1:G:366:ARG:HG2	1.99	0.44
1:B:389:LEU:CD1	1:B:437:VAL:HG12	2.47	0.44
1:G:296:LEU:CD2	1:G:347:TYR:CD2	3.00	0.44
1:C:482:VAL:CG1	1:C:484:ASP:O	2.66	0.44
1:B:456:MET:HE2	1:B:499:LEU:HD11	1.98	0.44
1:A:147:ILE:HA	1:A:150:ILE:HD12	1.99	0.44
1:G:128:ASP:HA	1:G:157:ILE:CD1	2.47	0.43
1:A:405:SER:CA	3:A:3282:HOH:O	2.66	0.43
1:A:27:ALA:N	3:A:1804:HOH:O	2.51	0.43
1:H:63:SER:HB2	3:H:1280:HOH:O	2.18	0.43
1:A:345:PRO:O	1:A:348:THR:HG22	2.17	0.43
1:F:242:THR:HG22	1:F:536:ARG:HB2	2.00	0.43
1:G:291:HIS:O	1:G:514:ALA:HA	2.18	0.43
1:H:195:LYS:HB3	3:H:1528:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:310:PHE:HD2	3:C:2179:HOH:O	1.93	0.43
1:B:300:TYR:CD1	1:B:505:ILE:HG23	2.53	0.43
1:F:347[A]:TYR:CD1	1:F:347[A]:TYR:N	2.85	0.43
1:D:296:LEU:HD23	1:D:347:TYR:CE2	2.53	0.43
1:G:521:VAL:HG22	3:G:3201:HOH:O	2.17	0.43
1:H:165:ILE:CD1	1:H:165:ILE:N	2.81	0.43
1:E:296:LEU:HD12	1:E:530:LEU:CD1	2.49	0.43
1:E:124:GLN:CG	1:E:157:ILE:HG23	2.48	0.43
1:E:349:ASP:O	1:E:449:PRO:HD3	2.17	0.43
1:G:340:ALA:HA	1:G:510:TYR:CE2	2.54	0.43
1:G:136:ALA:O	3:G:3275:HOH:O	2.21	0.43
1:C:176:GLU:HG3	1:C:177:PRO:HD2	2.00	0.43
1:E:109:SER:HA	1:E:235:THR:OG1	2.18	0.43
1:G:127:VAL:CB	3:G:3275:HOH:O	2.61	0.43
1:E:269:MET:HG3	3:E:1154:HOH:O	2.17	0.43
1:A:485:GLU:OE2	1:A:488:ARG:NH1	2.52	0.43
1:F:256:VAL:HG13	1:F:278:LEU:HD11	2.00	0.43
1:F:278:LEU:O	1:F:282:LEU:HG	2.19	0.43
1:H:60:VAL:N	1:H:61:PRO:CD	2.82	0.43
1:H:277:GLU:HG3	1:H:399:LYS:NZ	2.34	0.43
1:F:500:ASP:HB3	3:F:1241:HOH:O	2.19	0.43
1:C:472:PHE:CZ	3:C:3252:HOH:O	2.52	0.42
1:B:68:ASP:OD2	1:B:535:THR:HG23	2.19	0.42
1:D:69:LEU:HD21	1:D:230:LEU:HD22	2.00	0.42
1:H:143:HIS:CE1	1:H:480:LEU:HD11	2.53	0.42
1:A:405:SER:HA	3:A:3282:HOH:O	2.19	0.42
1:H:261:ARG:HD2	1:H:266:GLU:OE2	2.18	0.42
1:H:97:VAL:HG13	3:H:2194:HOH:O	2.18	0.42
1:G:488:ARG:NH2	3:G:2501:HOH:O	2.52	0.42
1:F:409:LYS:HG3	3:F:2305:HOH:O	2.18	0.42
1:H:59:GLY:HA3	1:H:62:GLU:OE1	2.20	0.42
1:C:310:PHE:CE1	1:C:319:LEU:CD1	3.03	0.42
1:A:490:ALA:O	1:A:493:THR:OG1	2.28	0.42
1:F:68:ASP:OD2	1:F:535[A]:THR:HG23	2.19	0.42
1:A:207:GLN:O	1:A:208:PRO:C	2.57	0.42
1:H:121:TYR:CB	1:H:195:LYS:HZ2	2.33	0.42
1:G:163:LYS:HD3	3:G:2241:HOH:O	2.18	0.42
1:F:387:ILE:HG22	1:F:416:VAL:HG13	2.00	0.42
1:E:313:VAL:HG11	1:G:314:ARG:HD2	2.02	0.42
1:H:128:ASP:HA	1:H:157:ILE:CD1	2.46	0.42
1:C:193:VAL:HG13	1:C:194:PRO:CD	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:232:ARG:HG3	1:E:242:THR:HG21	2.01	0.42
1:F:279:PHE:HB2	3:F:3260:HOH:O	2.19	0.42
1:C:127:VAL:O	1:C:127:VAL:HG12	2.19	0.42
1:F:386:THR:HG22	1:F:415:ASN:ND2	2.31	0.42
3:A:2316:HOH:O	1:C:313:VAL:HG22	2.19	0.42
1:B:300:TYR:HD1	1:B:505:ILE:HG23	1.85	0.42
1:F:277:GLU:HB2	3:F:2128:HOH:O	2.19	0.42
1:H:127:VAL:HG21	1:H:147:ILE:CD1	2.50	0.42
1:F:213:THR:HG1	1:F:218:THR:HG22	1.78	0.42
1:A:296:LEU:CD2	1:A:347:TYR:CD2	3.03	0.42
1:D:110:ASP:HB3	1:D:112:THR:H	1.85	0.42
3:D:3300:HOH:O	2:L:2:UNK:CB	2.68	0.42
1:E:310:PHE:HZ	1:E:387:ILE:CG2	2.33	0.42
1:E:310:PHE:HZ	1:E:387:ILE:HG21	1.84	0.42
1:A:140:GLN:NE2	3:A:558:HOH:O	2.52	0.42
1:B:300:TYR:CD1	1:B:505:ILE:HD12	2.55	0.42
1:F:329:VAL:HG23	1:F:509:TYR:HB3	2.01	0.42
1:G:127:VAL:HA	3:G:3275:HOH:O	2.19	0.42
1:A:485:GLU:OE1	1:A:488:ARG:HD2	2.20	0.42
1:D:37:GLU:CB	3:D:2127:HOH:O	2.68	0.42
1:G:385:LEU:HD11	1:G:387:ILE:HD11	2.02	0.42
1:C:261:ARG:HB2	1:C:267:ILE:HD12	2.02	0.42
1:G:538:MET:HE1	3:G:2372:HOH:O	2.19	0.41
1:D:55:HIS:O	1:D:133:SER:HB2	2.19	0.41
1:E:399:LYS:CE	3:E:2255:HOH:O	2.68	0.41
1:F:117:GLN:NE2	3:F:2475:HOH:O	2.53	0.41
1:A:292:VAL:HG13	1:A:512:VAL:HG13	2.01	0.41
1:E:92:ASN:HD22	1:E:95:ALA:H	1.68	0.41
1:A:323:MET:HA	1:A:323:MET:HE2	2.02	0.41
1:F:386:THR:O	1:F:387:ILE:HD12	2.20	0.41
1:G:51:SER:C	1:G:57:ILE:HD11	2.40	0.41
1:G:60:VAL:N	1:G:61:PRO:CD	2.83	0.41
1:H:274:MET:CE	1:H:279:PHE:HD2	2.33	0.41
1:G:385:LEU:HG	1:G:387:ILE:HD13	2.02	0.41
1:A:310:PHE:CE1	3:A:3257:HOH:O	2.57	0.41
1:E:69:LEU:O	1:E:213:THR:HB	2.20	0.41
1:B:310:PHE:HZ	1:B:387:ILE:HG21	1.85	0.41
1:D:273:SER:HB3	3:D:600:HOH:O	2.21	0.41
1:F:454:ASN:N	3:F:3223:HOH:O	2.54	0.41
1:H:52:LEU:HD12	1:H:222:TRP:CE3	2.56	0.41
1:F:55:HIS:CD2	1:F:125:ARG:HH21	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:367:ASN:O	1:F:370:ALA:HB3	2.21	0.41
1:H:260:ASN:ND2	3:H:1449:HOH:O	2.46	0.41
1:A:127:VAL:O	1:A:127:VAL:HG12	2.20	0.41
1:G:461:SER:HB3	3:G:2204:HOH:O	2.20	0.41
1:E:363:GLN:NE2	1:E:366:ARG:HH21	2.19	0.41
1:F:286:ILE:O	1:F:286:ILE:CG2	2.63	0.41
1:F:330:ASN:HB3	1:F:333:LYS:HZ2	1.86	0.41
1:B:123:TRP:CE3	1:B:162:VAL:HG21	2.52	0.41
1:C:424:LYS:HD2	3:C:756:HOH:O	2.20	0.41
1:G:274:MET:HE3	1:G:282:LEU:CD1	2.51	0.41
1:B:123:TRP:O	1:B:126[A]:SER:HB3	2.20	0.41
1:H:92:ASN:HD22	1:H:95:ALA:HA	1.85	0.41
1:C:50:GLN:HG2	1:C:424:LYS:HD2	2.03	0.41
1:A:45:ASN:ND2	1:A:64:ASN:HD22	2.19	0.41
1:A:166:ASP:HB2	3:A:1863:HOH:O	2.21	0.41
1:D:276:ILE:HG12	1:D:332:VAL:HG12	2.03	0.41
1:H:150:ILE:CG2	1:H:157:ILE:HD12	2.44	0.41
1:H:236:TYR:CE1	3:H:3291:HOH:O	2.71	0.41
1:G:168:HIS:CD2	3:G:958:HOH:O	2.74	0.41
1:F:196:ALA:HB3	3:F:1857:HOH:O	2.21	0.41
1:A:165:ILE:CD1	1:A:171:GLU:HB2	2.47	0.40
1:C:350:GLY:O	1:C:489:THR:CG2	2.69	0.40
1:B:324:ASP:CG	1:B:327:ILE:HD13	2.41	0.40
1:C:280:GLN:NE2	3:C:3302:HOH:O	2.51	0.40
1:E:127:VAL:HG13	1:E:150:ILE:CG2	2.52	0.40
1:C:317:THR:HG21	3:C:621:HOH:O	2.21	0.40
1:A:340:ALA:HA	1:A:510:TYR:CE2	2.56	0.40
1:B:28:ASP:OD1	1:B:241:LYS:NZ	2.44	0.40
1:E:340:ALA:HA	1:E:510:TYR:CE2	2.56	0.40
1:B:386:THR:HG22	1:B:415:ASN:ND2	2.33	0.40
1:B:286:ILE:CG2	1:B:289:GLU:HB2	2.51	0.40
1:F:540:ILE:N	1:F:540:ILE:HD12	2.36	0.40
1:H:352:LYS:HG3	3:H:2487:HOH:O	2.21	0.40
1:E:313:VAL:HG12	1:G:313:VAL:HG12	2.04	0.40
1:B:217:TYR:CE2	1:B:535:THR:OG1	2.75	0.40
1:B:286:ILE:HG21	1:B:289:GLU:CD	2.42	0.40
1:D:55:HIS:O	1:D:133:SER:CB	2.69	0.40
1:H:195:LYS:HG3	3:H:2094:HOH:O	2.21	0.40
1:G:42:VAL:HG22	1:G:248:THR:HB	2.02	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	517/524 (99%)	500 (97%)	15 (3%)	2 (0%)	39	33
1	B	517/524 (99%)	504 (98%)	12 (2%)	1 (0%)	52	48
1	C	516/524 (98%)	497 (96%)	18 (4%)	1 (0%)	52	48
1	D	516/524 (98%)	501 (97%)	14 (3%)	1 (0%)	52	48
1	E	517/524 (99%)	500 (97%)	16 (3%)	1 (0%)	52	48
1	F	519/524 (99%)	503 (97%)	15 (3%)	1 (0%)	52	48
1	G	517/524 (99%)	503 (97%)	13 (2%)	1 (0%)	52	48
1	H	516/524 (98%)	498 (96%)	16 (3%)	2 (0%)	39	33
All	All	4135/4192 (99%)	4006 (97%)	119 (3%)	10 (0%)	52	48

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	251	PRO
1	F	251	PRO
1	G	251	PRO
1	A	251	PRO
1	A	394	SER
1	C	251	PRO
1	E	251	PRO
1	H	251	PRO
1	H	394	SER
1	D	251	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	453/458 (99%)	442 (98%)	11 (2%)	57	58
1	B	453/458 (99%)	444 (98%)	9 (2%)	63	65
1	C	452/458 (99%)	447 (99%)	5 (1%)	80	83
1	D	452/458 (99%)	437 (97%)	15 (3%)	45	43
1	E	453/458 (99%)	446 (98%)	7 (2%)	72	75
1	F	455/458 (99%)	447 (98%)	8 (2%)	66	69
1	G	453/458 (99%)	441 (97%)	12 (3%)	54	54
1	H	452/458 (99%)	437 (97%)	15 (3%)	45	43
All	All	3623/3664 (99%)	3541 (98%)	82 (2%)	60	60

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	A	208	PRO
1	A	314	ARG
1	A	344	THR
1	A	348	THR
1	A	405	SER
1	A	439	ARG
1	A	474	SER
1	A	494	LYS
1	A	512	VAL
1	A	513	ASN
1	B	110	ASP
1	B	208	PRO
1	B	327	ILE
1	B	329	VAL
1	B	372	LYS
1	B	383	LYS
1	B	394	SER
1	B	439	ARG
1	B	474	SER
1	C	113	PRO
1	C	218	THR
1	C	346	PRO
1	C	439	ARG

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Mol	Chain	Res	Type
1	C	481	LYS
1	D	38	LYS
1	D	91	ASP
1	D	110	ASP
1	D	162	VAL
1	D	165	ILE
1	D	176	GLU
1	D	177	PRO
1	D	218	THR
1	D	233	SER
1	D	314	ARG
1	D	439	ARG
1	D	482	VAL
1	D	484	ASP
1	D	493	THR
1	D	513	ASN
1	E	91	ASP
1	E	127	VAL
1	E	176	GLU
1	E	220	LYS
1	E	357	GLU
1	E	439	ARG
1	E	513	ASN
1	F	38	LYS
1	F	157	ILE
1	F	329	VAL
1	F	347[A]	TYR
1	F	347[B]	TYR
1	F	396	LEU
1	F	439	ARG
1	F	512	VAL
1	G	38	LYS
1	G	57	ILE
1	G	110	ASP
1	G	133[A]	SER
1	G	133[B]	SER
1	G	157	ILE
1	G	221	ASP
1	G	255	GLU
1	G	406	SER
1	G	439	ARG
1	G	482	VAL

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Mol	Chain	Res	Type
1	G	512	VAL
1	H	91	ASP
1	H	99	THR
1	H	157	ILE
1	H	169	THR
1	H	203	GLU
1	H	208	PRO
1	H	221	ASP
1	H	233	SER
1	H	307	LYS
1	H	328	ILE
1	H	439	ARG
1	H	482	VAL
1	H	484	ASP
1	H	512	VAL
1	H	513	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	45	ASN
1	A	55	HIS
1	A	140	GLN
1	A	239	ASN
1	A	337	ASN
1	A	363	GLN
1	A	513	ASN
1	B	55	HIS
1	B	271	ASN
1	B	305	ASN
1	B	363	GLN
1	B	415	ASN
1	B	420	ASN
1	C	55	HIS
1	C	280	GLN
1	C	305	ASN
1	C	335	GLN
1	D	39	GLN
1	D	45	ASN
1	D	55	HIS
1	D	92	ASN

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Mol	Chain	Res	Type
1	D	140	GLN
1	D	239	ASN
1	D	246	GLN
1	D	363	GLN
1	D	513	ASN
1	E	39	GLN
1	E	45	ASN
1	E	55	HIS
1	E	92	ASN
1	E	239	ASN
1	E	305	ASN
1	E	363	GLN
1	E	432	GLN
1	E	487	GLN
1	E	513	ASN
1	F	39	GLN
1	F	45	ASN
1	F	55	HIS
1	F	117	GLN
1	F	140	GLN
1	F	239	ASN
1	F	246	GLN
1	F	305	ASN
1	F	363	GLN
1	F	432	GLN
1	F	513	ASN
1	G	39	GLN
1	G	45	ASN
1	G	55	HIS
1	G	140	GLN
1	G	207	GLN
1	G	239	ASN
1	G	246	GLN
1	G	280	GLN
1	G	363	GLN
1	G	432	GLN
1	G	513	ASN
1	H	39	GLN
1	H	45	ASN
1	H	92	ASN
1	H	140	GLN
1	H	239	ASN

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Mol	Chain	Res	Type
1	H	246	GLN
1	H	363	GLN
1	H	466	HIS
1	H	513	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 carbohydrates 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	517/524 (98%)	0.07	2 (0%) 93 93	14, 23, 36, 51	0
1	B	517/524 (98%)	0.31	35 (6%) 20 22	16, 28, 47, 61	0
1	C	517/524 (98%)	0.29	15 (2%) 55 56	19, 29, 42, 53	0
1	D	517/524 (98%)	0.27	13 (2%) 61 61	21, 30, 42, 53	0
1	E	517/524 (98%)	0.11	7 (1%) 78 78	17, 25, 36, 44	0
1	F	517/524 (98%)	0.34	24 (4%) 36 38	16, 25, 41, 57	0
1	G	517/524 (98%)	0.62	50 (9%) 10 10	17, 30, 51, 64	0
1	H	517/524 (98%)	0.92	94 (18%) 2 2	22, 38, 67, 79	0
2	I	0/3	-	-	-	-
2	J	0/3	-	-	-	-
2	K	0/3	-	-	-	-
2	L	0/3	-	-	-	-
2	M	0/3	-	-	-	-
2	N	0/3	-	-	-	-
2	O	0/3	-	-	-	-
2	P	0/3	-	-	-	-
All	All	4136/4216 (98%)	0.37	240 (5%) 26 28	14, 28, 48, 79	0

All (240) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	97	VAL	5.5
1	H	484	ASP	5.5
1	H	117	GLN	5.4
1	H	155	LYS	5.4
1	H	147	ILE	5.0
1	G	286	ILE	4.9
1	H	120	VAL	4.7
1	G	333	LYS	4.6

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Mol	Chain	Res	Type	RSRZ
1	F	275	PRO	4.6
1	H	483	THR	4.5
1	H	223	VAL	4.5
1	H	156	PRO	4.4
1	G	262	TYR	4.3
1	H	209	GLY	4.3
1	B	381	ALA	4.2
1	G	277	GLU	4.1
1	G	264	SER	4.0
1	H	193	VAL	4.0
1	H	158	THR	4.0
1	H	90	TRP	4.0
1	C	333	LYS	4.0
1	F	282	LEU	4.0
1	H	196	ALA	3.9
1	G	256	VAL	3.9
1	B	267	ILE	3.9
1	H	354	THR	3.9
1	F	259	VAL	3.9
1	H	144	ILE	3.9
1	H	164	ALA	3.9
1	B	334	ALA	3.8
1	G	543	HIS	3.8
1	D	483	THR	3.8
1	F	368	GLU	3.8
1	G	244	ILE	3.8
1	D	146	GLY	3.8
1	C	482	VAL	3.7
1	D	330	ASN	3.7
1	D	117	GLN	3.7
1	G	381	ALA	3.7
1	G	368	GLU	3.6
1	D	97	VAL	3.6
1	D	487	GLN	3.6
1	H	93	LYS	3.6
1	F	286	ILE	3.6
1	H	100	PHE	3.6
1	H	154	LYS	3.6
1	H	169	THR	3.5
1	C	97	VAL	3.5
1	G	267	ILE	3.5
1	G	276	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	H	150	ILE	3.5
1	G	259	VAL	3.5
1	H	86	VAL	3.5
1	H	166	ASP	3.5
1	H	165	ILE	3.5
1	B	364	GLU	3.4
1	F	277	GLU	3.4
1	H	126[A]	SER	3.4
1	B	370	ALA	3.4
1	H	203	GLU	3.4
1	B	284	LYS	3.4
1	E	333	LYS	3.4
1	H	333	LYS	3.4
1	H	124	GLN	3.4
1	B	286	ILE	3.4
1	D	484	ASP	3.4
1	H	224	VAL	3.4
1	G	265	GLY	3.3
1	G	252	ILE	3.3
1	G	287	PRO	3.3
1	B	368	GLU	3.3
1	H	347	TYR	3.3
1	H	162	VAL	3.3
1	E	364	GLU	3.3
1	C	165	ILE	3.3
1	H	122	SER	3.3
1	D	482	VAL	3.3
1	G	254	SER	3.3
1	B	383	LYS	3.2
1	B	382	ASP	3.2
1	H	157	ILE	3.2
1	H	197	ALA	3.2
1	H	173	THR	3.2
1	C	483	THR	3.1
1	H	204	LYS	3.1
1	B	520	TRP	3.1
1	H	366	ARG	3.1
1	G	258	ASP	3.1
1	H	94	ASP	3.1
1	H	178	VAL	3.1
1	G	280	GLN	3.1
1	G	33	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	334	ALA	3.0
1	H	361	TRP	3.0
1	E	360	GLY	3.0
1	G	290	VAL	3.0
1	G	410	LYS	3.0
1	D	94	ASP	3.0
1	H	167	ASP	3.0
1	H	359	PHE	3.0
1	B	384	PRO	2.9
1	F	347[A]	TYR	2.9
1	C	330	ASN	2.9
1	B	409	LYS	2.9
1	G	541	VAL	2.9
1	C	92	ASN	2.9
1	G	362	SER	2.9
1	B	256	VAL	2.9
1	B	406	SER	2.8
1	H	194	PRO	2.8
1	H	486	ALA	2.8
1	G	364	GLU	2.8
1	F	264	SER	2.8
1	G	279	PHE	2.8
1	B	258	ASP	2.8
1	F	364	GLU	2.8
1	C	93	LYS	2.8
1	H	98	TRP	2.8
1	B	265	GLY	2.8
1	G	382	ASP	2.8
1	B	333	LYS	2.7
1	H	487	GLN	2.7
1	H	201	PHE	2.7
1	D	490	ALA	2.7
1	F	284	LYS	2.7
1	H	357	GLU	2.7
1	G	407	LEU	2.7
1	H	160	LEU	2.7
1	C	95	ALA	2.7
1	B	278	LEU	2.6
1	H	210	ASN	2.6
1	H	171	GLU	2.6
1	H	130	ASN	2.6
1	H	230	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	415	ASN	2.6
1	G	409	LYS	2.6
1	F	254	SER	2.6
1	G	253	ALA	2.6
1	G	411	ASN	2.6
1	H	365	LYS	2.6
1	H	168	HIS	2.6
1	B	371	LYS	2.6
1	E	484	ASP	2.6
1	G	278	LEU	2.5
1	G	285	GLU	2.5
1	G	540	ILE	2.5
1	D	280	GLN	2.5
1	F	367	ASN	2.5
1	F	361	TRP	2.5
1	G	221	ASP	2.5
1	F	257	THR	2.5
1	F	258	ASP	2.5
1	H	465	ALA	2.4
1	F	382	ASP	2.4
1	G	520	TRP	2.4
1	G	37	GLU	2.4
1	G	284	LYS	2.4
1	H	481	LYS	2.4
1	A	541	VAL	2.4
1	H	368	GLU	2.4
1	E	330	ASN	2.4
1	B	226	GLU	2.4
1	B	410	LYS	2.4
1	H	99	THR	2.4
1	H	131	THR	2.4
1	B	367	ASN	2.4
1	H	108	TRP	2.4
1	C	117	GLN	2.4
1	F	343	TYR	2.4
1	F	329	VAL	2.4
1	B	542	LYS	2.4
1	G	226	GLU	2.4
1	H	174	LEU	2.4
1	A	382	ASP	2.3
1	H	60	VAL	2.3
1	G	38	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	486	ALA	2.3
1	H	330	ASN	2.3
1	F	334	ALA	2.3
1	G	542	LYS	2.3
1	H	370	ALA	2.3
1	G	260	ASN	2.3
1	B	257	THR	2.3
1	H	218	THR	2.3
1	B	375	ALA	2.3
1	F	409	LYS	2.3
1	H	163	LYS	2.3
1	G	330	ASN	2.3
1	H	143	HIS	2.3
1	H	127	VAL	2.3
1	B	344	THR	2.3
1	B	260	ASN	2.3
1	F	365	LYS	2.3
1	E	280	GLN	2.2
1	H	141	TYR	2.2
1	H	177	PRO	2.2
1	F	267	ILE	2.2
1	H	119	PHE	2.2
1	H	467	TYR	2.2
1	C	96	LYS	2.2
1	B	363	GLN	2.2
1	G	167	ASP	2.2
1	G	396	LEU	2.2
1	H	353	LEU	2.2
1	D	93	LYS	2.2
1	G	519	PRO	2.2
1	F	278	LEU	2.2
1	G	499	LEU	2.2
1	B	322	GLY	2.2
1	C	70	PHE	2.2
1	F	449	PRO	2.2
1	H	208	PRO	2.2
1	H	159	ASP	2.1
1	C	410	LYS	2.1
1	H	329	VAL	2.1
1	H	221	ASP	2.1
1	B	362	SER	2.1
1	E	361	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	31	ALA	2.1
1	G	343	TYR	2.1
1	H	142	GLY	2.1
1	D	535	THR	2.1
1	H	352	LYS	2.1
1	H	482	VAL	2.1
1	H	453	LEU	2.1
1	H	129	PRO	2.1
1	H	363	GLN	2.1
1	H	38	LYS	2.1
1	H	95	ALA	2.1
1	H	422	GLU	2.0
1	H	151	LEU	2.0
1	C	94	ASP	2.0
1	H	191	SER	2.0
1	B	266	GLU	2.0
1	B	277	GLU	2.0
1	B	288	ASP	2.0
1	H	326	ASP	2.0
1	H	280	GLN	2.0
1	H	172	VAL	2.0
1	H	428	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.