



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2024 – 04:50 PM EST

PDB ID : 3TCG
Title : Crystal structure of E. coli OppA complexed with the tripeptide KGE
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

<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	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

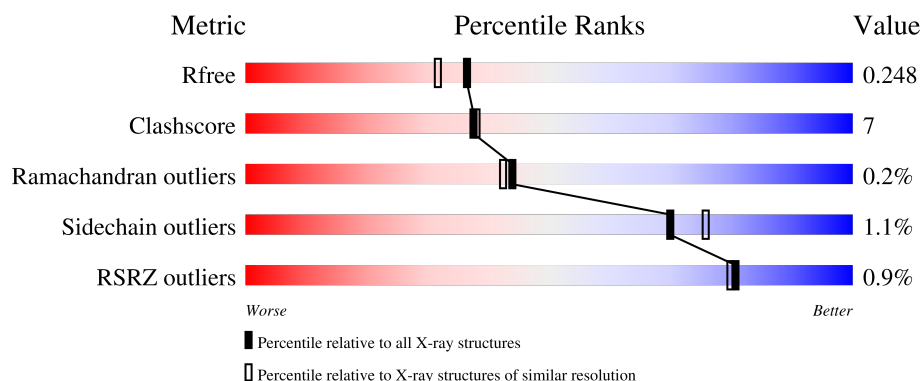
1 Overall quality at a glance

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}	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (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 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	524	<div> <div>88%</div> <div>10%</div> <div>.</div> </div>
1	B	524	<div> <div>89%</div> <div>9%</div> <div>.</div> </div>
1	C	524	<div> <div>88%</div> <div>10%</div> <div>.</div> </div>
1	D	524	<div> <div>%</div> <div>87%</div> <div>11%</div> <div>.</div> </div>
1	E	524	<div> <div>%</div> <div>87%</div> <div>11%</div> <div>.</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	524	 85% 13%
1	G	524	 85% 13%
1	H	524	 4% 85% 14%
2	I	3	 67% 33%
2	J	3	 67% 33%
2	K	3	 67% 33%
2	L	3	 67% 33%
2	M	3	 67% 33%
2	N	3	 67% 33%
2	O	3	 33% 67%
2	P	3	 67% 33%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 36270 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	3	0
			4141	2641	694	796	10			
1	B	517	Total	C	N	O	S	0	4	0
			4150	2646	696	798	10			
1	C	517	Total	C	N	O	S	0	3	0
			4141	2641	694	796	10			
1	D	517	Total	C	N	O	S	0	4	0
			4150	2646	696	798	10			
1	E	517	Total	C	N	O	S	0	4	0
			4148	2646	695	797	10			
1	F	517	Total	C	N	O	S	0	2	0
			4129	2632	693	794	10			
1	G	517	Total	C	N	O	S	0	3	0
			4135	2635	694	796	10			
1	H	517	Total	C	N	O	S	6	3	0
			4141	2641	694	796	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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	549	HIS	-	expression tag	UNP P23843

- Molecule 2 is a protein called KGE Peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	3	Total	C	N	O	0	0	0
			22	13	4	5			
2	J	3	Total	C	N	O	0	0	0
			22	13	4	5			
2	K	3	Total	C	N	O	0	0	0
			22	13	4	5			
2	L	3	Total	C	N	O	0	0	0
			22	13	4	5			
2	M	3	Total	C	N	O	0	0	0
			22	13	4	5			
2	N	3	Total	C	N	O	0	0	0
			22	13	4	5			
2	O	3	Total	C	N	O	0	0	0
			22	13	4	5			
2	P	3	Total	C	N	O	0	0	0
			22	13	4	5			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	398	Total	O	0	0
			398	398		
3	B	347	Total	O	0	0
			347	347		
3	C	430	Total	O	0	0
			430	430		
3	D	366	Total	O	0	0
			366	366		
3	E	408	Total	O	0	0
			408	408		
3	F	359	Total	O	0	0
			359	359		
3	G	349	Total	O	0	0
			349	349		
3	H	279	Total	O	0	0
			279	279		
3	I	3	Total	O	0	0
			3	3		

Continued on next page...


Continued from previous page...

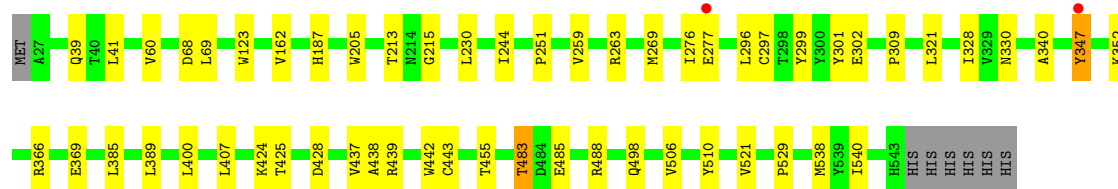
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	3	Total 3	O 3	0	0
3	K	2	Total 2	O 2	0	0
3	L	3	Total 3	O 3	0	0
3	M	2	Total 2	O 2	0	0
3	N	4	Total 4	O 4	0	0
3	O	2	Total 2	O 2	0	0
3	P	4	Total 4	O 4	0	0

3 Residue-property plots


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.

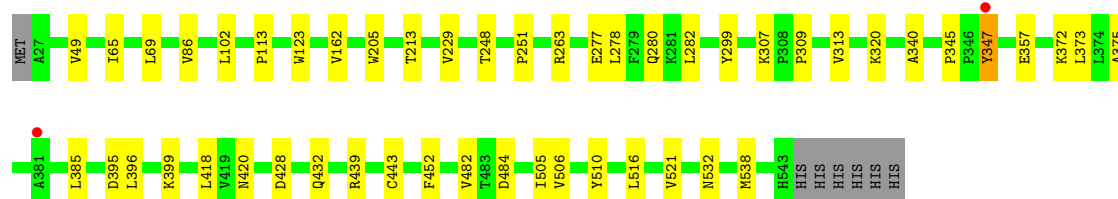
• Molecule 1: Periplasmic oligopeptide-binding protein

Chain A: 




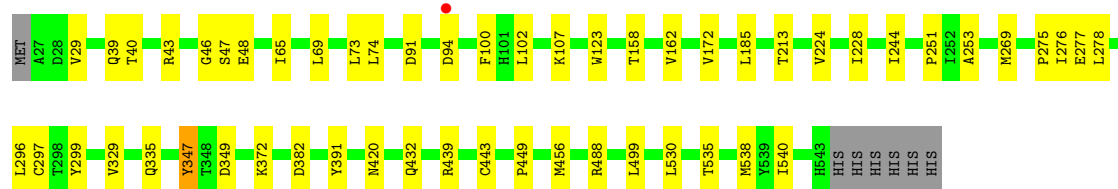
• Molecule 1: Periplasmic oligopeptide-binding protein

Chain B: 




• Molecule 1: Periplasmic oligopeptide-binding protein

Chain C: 



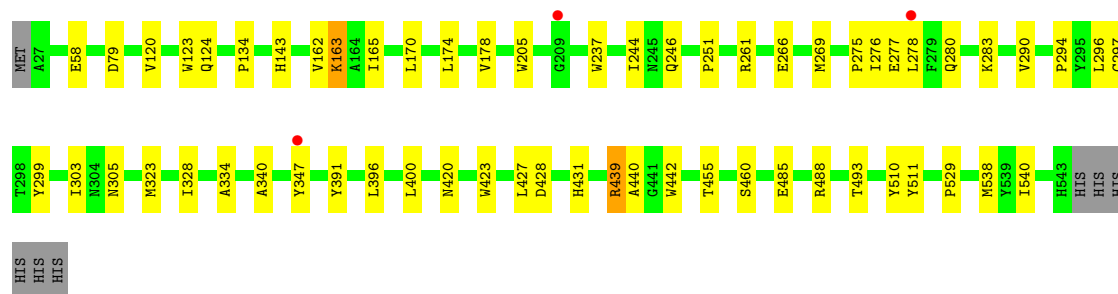
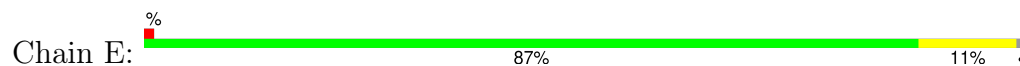
• Molecule 1: Periplasmic oligopeptide-binding protein

Chain D: 

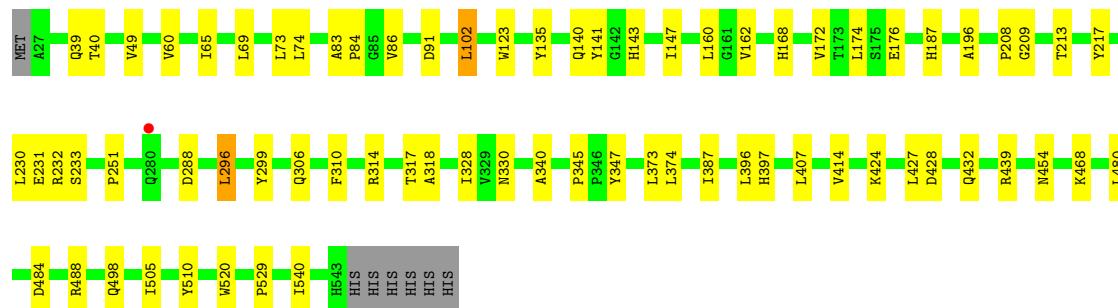
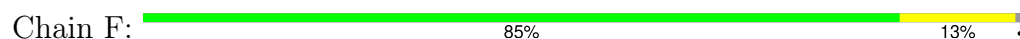




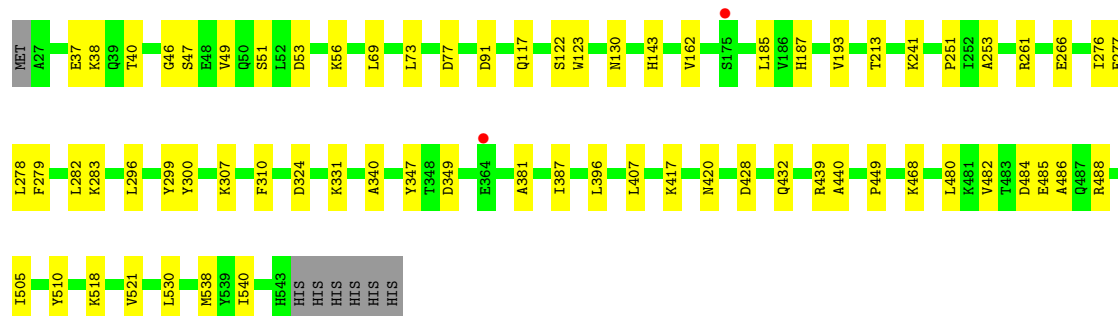
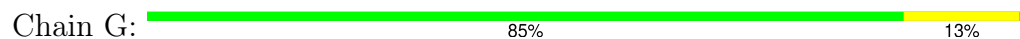
- Molecule 1: Periplasmic oligopeptide-binding protein



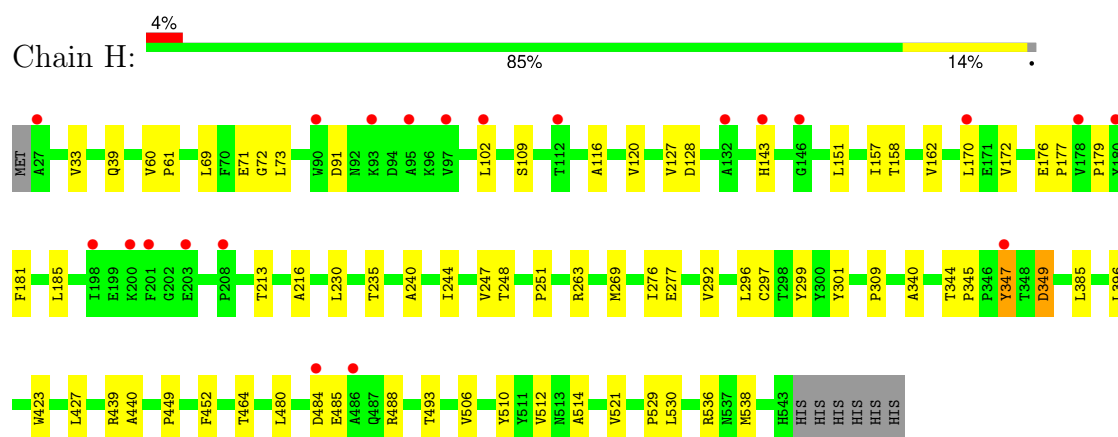
- Molecule 1: Periplasmic oligopeptide-binding protein



- Molecule 1: Periplasmic oligopeptide-binding protein



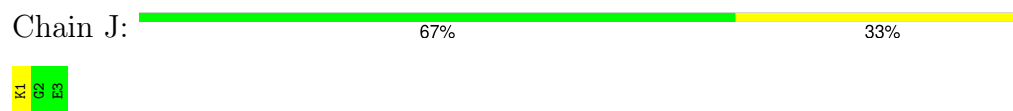
- Molecule 1: Periplasmic oligopeptide-binding protein



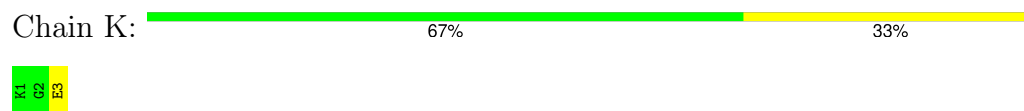
- Molecule 2: KGE Peptide



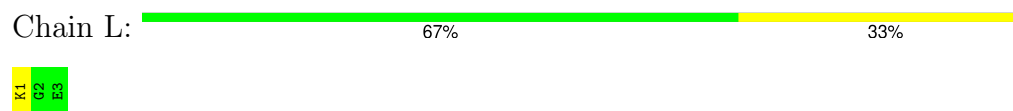
- Molecule 2: KGE Peptide



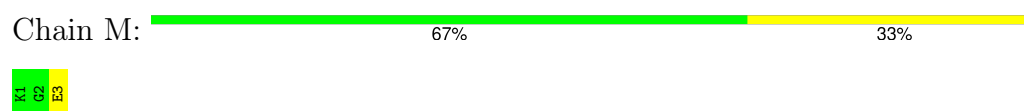
- Molecule 2: KGE Peptide



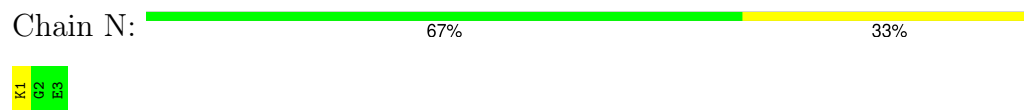
- Molecule 2: KGE Peptide



- Molecule 2: KGE Peptide



- Molecule 2: KGE Peptide



- Molecule 2: KGE Peptide

Chain O:  33% 67%

 K1 G2 E3

● Molecule 2: KGE Peptide

Chain P:  67% 33%

 K1 G2 E3

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.49Å 201.31Å 206.95Å 90.00° 95.57° 90.00°	Depositor
Resolution (Å)	48.89 – 2.00 48.89 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.89-2.00) 99.7 (48.89-2.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 2.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.199 , 0.245 0.203 , 0.248	Depositor DCC
R_{free} test set	17044 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	20.1	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	36270	wwPDB-VP
Average B, all atoms (Å ²)	25.0	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 20.49 % 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 8.5943e-03.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.62	2/4250 (0.0%)	0.63	0/5797
1	B	0.58	1/4259 (0.0%)	0.62	0/5809
1	C	0.59	0/4250	0.63	0/5797
1	D	0.59	1/4259 (0.0%)	0.61	0/5809
1	E	0.61	3/4257 (0.1%)	0.62	0/5807
1	F	0.58	1/4237 (0.0%)	0.59	0/5779
1	G	0.58	0/4243	0.60	0/5787
1	H	0.57	0/4250	0.58	0/5797
2	I	0.54	0/21	0.81	0/25
2	J	0.71	0/21	0.71	0/25
2	K	0.69	0/21	0.77	0/25
2	L	0.92	0/21	0.61	0/25
2	M	0.59	0/21	0.64	0/25
2	N	0.60	0/21	0.76	0/25
2	O	0.52	0/21	0.50	0/25
2	P	0.45	0/21	0.48	0/25
All	All	0.59	8/34173 (0.0%)	0.61	0/46582

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	442	TRP	CD2-CE2	6.01	1.48	1.41
1	A	205	TRP	CD2-CE2	5.21	1.47	1.41
1	B	205	TRP	CD2-CE2	5.16	1.47	1.41
1	D	205	TRP	CD2-CE2	5.15	1.47	1.41
1	E	205	TRP	CD2-CE2	5.14	1.47	1.41
1	F	520	TRP	CD2-CE2	5.13	1.47	1.41
1	E	237	TRP	CD2-CE2	5.05	1.47	1.41
1	E	442	TRP	CD2-CE2	5.02	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4141	0	4047	53	0
1	B	4150	0	4054	37	0
1	C	4141	0	4047	49	0
1	D	4150	0	4054	50	0
1	E	4148	0	4055	70	0
1	F	4129	0	4039	61	0
1	G	4135	0	4043	70	0
1	H	4141	0	4047	61	0
2	I	22	0	24	2	0
2	J	22	0	24	0	0
2	K	22	0	24	0	0
2	L	22	0	24	4	0
2	M	22	0	24	1	0
2	N	22	0	24	1	0
2	O	22	0	24	1	0
2	P	22	0	24	1	0
3	A	398	0	0	22	0
3	B	347	0	0	17	0
3	C	430	0	0	27	0
3	D	366	0	0	31	0
3	E	408	0	0	44	0
3	F	359	0	0	31	0
3	G	349	0	0	44	0
3	H	279	0	0	31	0
3	I	3	0	0	1	0
3	J	3	0	0	0	0
3	K	2	0	0	0	0
3	L	3	0	0	0	0
3	M	2	0	0	0	0
3	N	4	0	0	0	0
3	O	2	0	0	1	0
3	P	4	0	0	1	0
All	All	36270	0	32578	455	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 7.

All (455) 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:303:ILE:HG22	3:E:3206:HOH:O	1.27	1.28
1:C:224:VAL:HG13	3:C:3004:HOH:O	1.14	1.27
1:C:158:THR:HG23	3:C:2936:HOH:O	1.33	1.27
1:F:217:TYR:HA	3:F:2653:HOH:O	1.30	1.26
1:A:297:CYS:HB3	3:A:2899:HOH:O	1.33	1.24
1:F:427:LEU:HD12	3:F:3226:HOH:O	1.25	1.23
1:F:160:LEU:HD23	3:F:2398:HOH:O	1.32	1.22
1:A:437:VAL:HG13	3:A:2590:HOH:O	1.35	1.21
1:B:229:VAL:HG22	3:B:2652:HOH:O	1.40	1.19
1:G:407:LEU:HD13	3:G:2505:HOH:O	1.43	1.18
1:H:216:ALA:HB2	3:H:2444:HOH:O	1.44	1.14
1:C:297:CYS:HB3	3:C:2905:HOH:O	1.46	1.14
1:C:213:THR:HG21	3:C:3079:HOH:O	1.51	1.11
1:H:247:VAL:HG22	3:H:2516:HOH:O	1.48	1.10
1:D:162:VAL:HG13	3:D:3002:HOH:O	1.53	1.09
1:G:49:VAL:HG12	3:G:2578:HOH:O	0.89	1.06
1:F:306:GLN:HA	3:F:2774:HOH:O	1.55	1.03
1:C:244:ILE:HG12	3:C:1035:HOH:O	1.56	1.02
1:H:297:CYS:HB3	3:H:2918:HOH:O	1.56	1.02
1:F:414:VAL:HG13	3:F:2546:HOH:O	1.60	1.01
1:G:40:THR:O	1:G:540:ILE:HD11	1.60	1.01
3:E:2672:HOH:O	2:M:3:GLU:C	1.99	1.00
1:E:334:ALA:HB3	3:E:3157:HOH:O	1.62	0.99
1:D:121:TYR:HA	3:D:2490:HOH:O	1.62	0.99
1:A:68:ASP:O	3:A:2692:HOH:O	1.83	0.97
1:E:120:VAL:O	3:E:2640:HOH:O	1.84	0.95
1:H:33:VAL:HG12	3:H:3220:HOH:O	1.66	0.95
1:E:123:TRP:N	3:E:2640:HOH:O	1.99	0.94
1:E:174:LEU:HB3	3:E:3073:HOH:O	1.67	0.94
1:H:493:THR:HG21	3:H:1916:HOH:O	1.68	0.93
1:G:440:ALA:HB3	3:G:2521:HOH:O	1.68	0.92
1:E:134:PRO:CB	3:E:2832:HOH:O	2.18	0.91
1:E:460:SER:HB3	3:E:2784:HOH:O	1.71	0.91
1:F:160:LEU:CD2	3:F:2398:HOH:O	1.96	0.90
1:C:102:LEU:HG	3:C:2541:HOH:O	1.70	0.90
1:E:493:THR:HG22	3:E:2986:HOH:O	1.72	0.89
1:G:540:ILE:HG12	3:G:1438:HOH:O	1.70	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:317:THR:HB	3:F:2710:HOH:O	1.72	0.88
1:G:428[A]:ASP:HB3	3:G:2354:HOH:O	1.71	0.88
1:C:69:LEU:HD22	3:C:3079:HOH:O	1.74	0.87
1:H:162:VAL:CG2	3:H:2655:HOH:O	2.23	0.87
2:P:1:LYS:NZ	3:P:2879:HOH:O	2.06	0.87
1:E:455:THR:C	3:E:2784:HOH:O	2.11	0.86
1:G:407:LEU:CD1	3:G:2505:HOH:O	2.11	0.85
1:E:134:PRO:HB3	3:E:2832:HOH:O	1.75	0.85
1:A:296:LEU:HD13	1:A:529:PRO:HB2	1.57	0.84
1:F:428[A]:ASP:HB3	3:F:2377:HOH:O	1.77	0.83
1:H:512:VAL:HG23	3:H:2459:HOH:O	1.79	0.82
1:E:244:ILE:HD11	3:E:2695:HOH:O	1.79	0.81
1:A:297:CYS:CB	3:A:2899:HOH:O	2.07	0.80
1:C:40:THR:O	1:C:540:ILE:HD11	1.82	0.80
1:F:232:ARG:HA	3:F:2653:HOH:O	1.81	0.79
1:D:124:GLN:NE2	3:D:2490:HOH:O	2.15	0.79
1:D:455:THR:HA	3:D:2543:HOH:O	1.82	0.78
1:F:314:ARG:HA	3:F:2710:HOH:O	1.82	0.78
1:D:466:HIS:CD2	3:D:3188:HOH:O	2.34	0.78
1:A:437:VAL:HG12	3:A:2573:HOH:O	1.81	0.78
1:D:455:THR:HG22	3:D:2543:HOH:O	1.82	0.78
1:E:455:THR:O	3:E:2784:HOH:O	2.01	0.78
1:C:47:SER:HA	3:C:2514:HOH:O	1.85	0.76
1:H:69:LEU:HD21	1:H:230:LEU:HD22	1.66	0.76
1:H:514:ALA:HB2	3:H:2459:HOH:O	1.86	0.76
1:B:428[A]:ASP:HB3	3:B:926:HOH:O	1.85	0.76
1:A:302:GLU:O	3:A:2590:HOH:O	2.05	0.74
1:H:240:ALA:HB3	3:H:3219:HOH:O	1.87	0.74
1:G:53:ASP:O	3:G:2800:HOH:O	2.07	0.73
1:E:134:PRO:HB2	3:E:2832:HOH:O	1.82	0.73
1:F:498:GLN:OE1	3:F:2320:HOH:O	2.07	0.72
1:C:46:GLY:O	3:C:2514:HOH:O	2.07	0.72
1:C:443:CYS:SG	3:C:2905:HOH:O	2.47	0.72
1:G:396:LEU:HG	3:G:3241:HOH:O	1.90	0.72
1:D:120:VAL:HG13	3:D:3002:HOH:O	1.90	0.71
1:F:396:LEU:HD13	1:F:396:LEU:C	2.12	0.71
1:G:47:SER:HA	3:G:2420:HOH:O	1.90	0.70
1:C:443:CYS:HB3	3:C:2943:HOH:O	1.90	0.70
1:G:122:SER:HA	3:G:2762:HOH:O	1.91	0.70
1:G:296:LEU:HD12	1:G:530:LEU:CD1	2.21	0.70
1:G:300:TYR:CG	3:G:2521:HOH:O	2.45	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:CYS:CB	3:C:2905:HOH:O	2.18	0.69
1:E:244:ILE:CG1	3:E:2695:HOH:O	2.40	0.69
1:E:529:PRO:HB3	3:E:2603:HOH:O	1.91	0.69
1:F:40:THR:O	1:F:540:ILE:HD11	1.91	0.69
1:F:296:LEU:HD12	1:F:347:TYR:CE1	2.27	0.69
1:C:335:GLN:NE2	3:C:2419:HOH:O	2.25	0.69
1:C:100:PHE:O	3:C:2541:HOH:O	2.12	0.68
1:B:505:ILE:HG22	3:B:1731:HOH:O	1.93	0.68
1:B:248:THR:HG23	3:B:2652:HOH:O	1.95	0.67
1:F:432:GLN:NE2	3:F:2377:HOH:O	2.25	0.67
1:H:170:LEU:HD11	3:H:2311:HOH:O	1.94	0.67
1:H:452:PHE:HB3	3:H:2538:HOH:O	1.95	0.67
1:F:414:VAL:CG1	3:F:2546:HOH:O	2.26	0.67
1:G:278:LEU:HD12	3:G:2944:HOH:O	1.94	0.66
1:A:276:ILE:HD11	1:A:400:LEU:HD11	1.79	0.65
1:G:310:PHE:HZ	1:G:387:ILE:HG21	1.62	0.65
1:E:244:ILE:HG12	3:E:2695:HOH:O	1.97	0.65
1:H:71:GLU:HA	3:H:1473:HOH:O	1.95	0.65
1:F:232:ARG:CA	3:F:2653:HOH:O	2.40	0.65
1:C:29:VAL:HG23	3:C:2797:HOH:O	1.97	0.65
1:G:143:HIS:NE2	1:G:480:LEU:HD11	2.12	0.64
1:G:324:ASP:HB3	3:G:2505:HOH:O	1.97	0.64
1:H:269:MET:SD	1:H:538:MET:HE1	2.38	0.64
1:D:141:TYR:OH	3:D:2543:HOH:O	1.79	0.64
1:E:163:LYS:N	3:E:2511:HOH:O	2.30	0.64
1:D:47:SER:CB	3:D:3190:HOH:O	2.45	0.64
1:E:244:ILE:CD1	3:E:2695:HOH:O	2.39	0.64
1:B:482:VAL:HG23	3:B:1039:HOH:O	1.98	0.63
1:G:300:TYR:CD2	3:G:2521:HOH:O	2.51	0.63
1:B:123:TRP:HE3	1:B:162:VAL:HG11	1.62	0.63
1:H:521:VAL:HG13	1:H:538:MET:HE3	1.81	0.63
1:G:505:ILE:HG22	3:G:3075:HOH:O	1.99	0.63
1:H:296:LEU:HD13	1:H:529:PRO:HB2	1.79	0.63
1:D:375:ALA:HB3	3:D:1567:HOH:O	1.99	0.62
1:F:296:LEU:HB3	3:F:3173:HOH:O	2.00	0.62
1:A:443:CYS:HB3	3:I:1663:HOH:O	1.99	0.61
1:E:170:LEU:CD1	3:E:2511:HOH:O	2.47	0.61
1:H:151:LEU:HA	3:H:2702:HOH:O	2.01	0.61
1:E:269:MET:SD	1:E:538:MET:HE1	2.40	0.61
1:G:193:VAL:CG2	3:G:2762:HOH:O	2.47	0.61
1:H:521:VAL:CG1	1:H:538:MET:HE3	2.31	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:TRP:HE3	1:C:162:VAL:HG11	1.65	0.61
1:G:440:ALA:CB	3:G:2521:HOH:O	2.39	0.61
1:H:102:LEU:HD13	3:H:2545:HOH:O	2.01	0.60
1:H:143:HIS:NE2	1:H:480:LEU:HD11	2.16	0.60
1:F:310:PHE:HZ	1:F:387:ILE:HG21	1.66	0.60
1:A:215:GLY:CA	3:A:2692:HOH:O	2.50	0.60
1:G:73:LEU:HD12	1:G:185:LEU:HD13	1.82	0.59
1:A:41:LEU:HB2	1:A:244:ILE:HD13	1.84	0.59
1:D:124:GLN:HB2	3:D:2490:HOH:O	2.01	0.59
1:G:396:LEU:CD1	3:G:3241:HOH:O	2.50	0.59
1:D:347[A]:TYR:N	1:D:347[A]:TYR:CD2	2.70	0.59
1:F:123:TRP:HE3	1:F:162:VAL:HG11	1.66	0.59
1:H:345:PRO:HB2	3:H:2840:HOH:O	2.01	0.59
1:C:39:GLN:HA	1:C:540:ILE:HD12	1.83	0.59
1:G:440:ALA:C	3:G:2521:HOH:O	2.40	0.59
1:A:483:THR:HG22	3:A:1078:HOH:O	2.03	0.59
1:E:396:LEU:CD1	1:E:400:LEU:HD22	2.33	0.59
1:B:123:TRP:CE3	1:B:162:VAL:HG11	2.38	0.59
1:E:303:ILE:CG2	3:E:3206:HOH:O	2.07	0.59
1:A:215:GLY:HA3	3:A:2692:HOH:O	2.03	0.59
1:D:386:THR:HG21	3:D:2390:HOH:O	2.03	0.58
1:B:86:VAL:HG12	1:B:102:LEU:HD22	1.84	0.58
1:G:396:LEU:CG	3:G:3241:HOH:O	2.49	0.58
1:A:330:ASN:HB3	3:A:2766:HOH:O	2.02	0.58
1:E:431:HIS:NE2	3:E:2832:HOH:O	2.32	0.58
1:A:437:VAL:CG1	3:A:2573:HOH:O	2.45	0.58
1:C:107:LYS:NZ	3:C:3232:HOH:O	2.36	0.58
1:E:278:LEU:HD23	3:E:2705:HOH:O	2.03	0.57
1:H:263:ARG:CZ	3:H:2627:HOH:O	2.52	0.57
1:D:296:LEU:HD13	1:D:529:PRO:HB2	1.86	0.57
1:E:170:LEU:HD12	3:E:2511:HOH:O	2.02	0.57
1:F:143:HIS:NE2	1:F:480:LEU:HD11	2.18	0.57
1:H:344:THR:N	3:H:2538:HOH:O	2.35	0.57
1:B:277:GLU:HB2	1:B:278:LEU:HD12	1.86	0.57
1:F:231:GLU:O	3:F:2653:HOH:O	2.16	0.57
1:D:49:VAL:HG23	3:D:3239:HOH:O	2.04	0.57
1:C:269:MET:SD	1:C:538:MET:HE1	2.44	0.57
1:E:347[B]:TYR:CD2	1:E:347[B]:TYR:N	2.73	0.56
1:B:347[A]:TYR:N	1:B:347[A]:TYR:CD2	2.71	0.56
1:B:432:GLN:NE2	3:B:926:HOH:O	2.38	0.56
1:F:387:ILE:HG23	3:F:2546:HOH:O	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:LEU:HD22	3:B:3131:HOH:O	2.05	0.56
1:D:340:ALA:HA	1:D:510:TYR:CE2	2.40	0.56
1:G:486:ALA:HB3	3:G:2641:HOH:O	2.05	0.56
1:F:143:HIS:CD2	1:F:480:LEU:HD11	2.41	0.56
1:H:248:THR:C	3:H:2516:HOH:O	2.44	0.55
1:A:215:GLY:C	3:A:2692:HOH:O	2.43	0.55
1:C:382:ASP:HB3	3:C:1130:HOH:O	2.05	0.55
1:E:296:LEU:HD23	1:E:347[B]:TYR:CE1	2.41	0.55
1:F:396:LEU:HD12	1:F:397:HIS:ND1	2.22	0.55
1:A:276:ILE:HD11	1:A:400:LEU:CD1	2.37	0.55
1:G:277:GLU:HB3	1:G:278:LEU:HD12	1.89	0.55
1:C:269:MET:SD	1:C:538:MET:CE	2.95	0.55
1:B:299:TYR:CZ	1:B:439:ARG:HD3	2.42	0.55
1:A:340:ALA:HA	1:A:510:TYR:CE2	2.42	0.55
1:C:40:THR:O	1:C:540:ILE:CD1	2.54	0.54
1:B:307:LYS:HE3	3:B:2056:HOH:O	2.07	0.54
1:C:46:GLY:C	3:C:2514:HOH:O	2.44	0.54
1:C:372:LYS:NZ	3:C:1162:HOH:O	2.41	0.54
1:B:357:GLU:HB2	3:B:2611:HOH:O	2.07	0.54
1:G:396:LEU:HD12	3:G:3241:HOH:O	2.06	0.54
1:A:296:LEU:CD1	1:A:529:PRO:HB2	2.32	0.54
1:E:347[A]:TYR:CE2	3:E:3179:HOH:O	2.53	0.54
1:F:424:LYS:HA	3:F:3226:HOH:O	2.08	0.54
1:A:425:THR:HB	3:A:2381:HOH:O	2.07	0.54
2:O:1:LYS:NZ	3:O:2875:HOH:O	2.17	0.54
1:B:229:VAL:CG2	3:B:2652:HOH:O	2.18	0.53
1:G:484:ASP:OD1	1:G:485:GLU:N	2.42	0.53
1:D:296:LEU:HD12	1:D:347[A]:TYR:CE1	2.44	0.53
1:D:326:ASP:O	1:D:330:ASN:ND2	2.41	0.53
1:A:296:LEU:HD12	1:A:347[A]:TYR:CE1	2.43	0.53
1:A:498:GLN:NE2	3:A:2649:HOH:O	2.41	0.53
1:D:47:SER:HB2	3:D:3190:HOH:O	2.07	0.53
1:G:123:TRP:HE3	1:G:162:VAL:HG11	1.74	0.53
1:A:521:VAL:CG1	1:A:538:MET:CE	2.87	0.52
1:D:60:VAL:HG22	2:L:1:LYS:HE3	1.91	0.52
1:E:123:TRP:HE3	1:E:162[A]:VAL:HG11	1.74	0.52
1:F:328:ILE:HD11	1:F:407:LEU:HD12	1.92	0.52
1:H:116:ALA:O	1:H:120:VAL:HG23	2.10	0.52
1:D:462:MET:HB2	3:D:2543:HOH:O	2.09	0.52
1:D:498:GLN:CD	3:D:1244:HOH:O	2.47	0.52
1:G:261:ARG:HD2	1:G:266:GLU:OE2	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:162:VAL:HG23	3:H:2655:HOH:O	2.01	0.52
1:C:299:TYR:CZ	1:C:439:ARG:HD3	2.45	0.52
1:E:294:PRO:HB2	3:E:2603:HOH:O	2.10	0.52
1:F:162:VAL:HG12	1:F:172:VAL:HG13	1.91	0.52
1:G:396:LEU:HD13	1:G:396:LEU:C	2.30	0.52
1:G:46:GLY:C	3:G:2420:HOH:O	2.48	0.52
1:E:246:GLN:HG2	3:E:2997:HOH:O	2.09	0.52
1:E:396:LEU:HD11	1:E:400:LEU:HD22	1.92	0.52
1:F:49:VAL:HG11	1:F:65:ILE:HD12	1.91	0.52
1:G:349:ASP:O	1:G:449:PRO:HD3	2.10	0.52
1:G:521:VAL:CG1	1:G:538:MET:HE2	2.39	0.52
1:H:296:LEU:HG	3:H:2840:HOH:O	2.10	0.52
1:C:43:ARG:CZ	3:C:2345:HOH:O	2.57	0.51
1:C:244:ILE:HD12	1:C:535:THR:O	2.10	0.51
1:F:69:LEU:HD21	1:F:230:LEU:HD22	1.91	0.51
1:E:299:TYR:CZ	1:E:439:ARG:HD3	2.45	0.51
1:D:485:GLU:CD	1:D:488:ARG:NH1	2.64	0.51
1:E:120:VAL:C	3:E:2640:HOH:O	2.42	0.51
1:A:187:HIS:CE1	3:A:2384:HOH:O	2.64	0.51
1:B:49:VAL:HG11	1:B:65:ILE:HD12	1.92	0.51
1:E:174:LEU:HD13	3:E:3073:HOH:O	2.10	0.51
1:C:73:LEU:HD12	1:C:185:LEU:HD13	1.92	0.51
1:E:296:LEU:HD23	1:E:347[B]:TYR:CD1	2.46	0.51
1:F:488:ARG:NH2	3:F:2580:HOH:O	2.44	0.51
1:A:347[A]:TYR:CD2	1:A:347[A]:TYR:N	2.78	0.51
1:B:320:LYS:HA	1:B:506:VAL:HG13	1.93	0.51
1:D:226:GLU:HB2	3:D:1295:HOH:O	2.11	0.51
1:G:56:LYS:HB2	3:G:2800:HOH:O	2.10	0.51
3:D:2141:HOH:O	1:H:235:THR:HG23	2.11	0.50
1:H:536:ARG:HD3	3:H:2444:HOH:O	2.10	0.50
1:A:269:MET:SD	1:A:538:MET:CE	2.99	0.50
1:A:299:TYR:CZ	1:A:439:ARG:HD3	2.46	0.50
1:D:485:GLU:OE2	1:D:488:ARG:NH1	2.45	0.50
1:C:253:ALA:N	3:C:2514:HOH:O	2.44	0.50
1:F:340:ALA:HA	1:F:510:TYR:CE2	2.47	0.50
1:F:299:TYR:CZ	1:F:439:ARG:HD3	2.46	0.50
1:G:518:LYS:HE2	3:G:3154:HOH:O	2.11	0.50
1:G:187:HIS:HE1	3:G:2919:HOH:O	1.95	0.50
1:A:60:VAL:HG22	2:I:1:LYS:HD2	1.94	0.50
1:F:396:LEU:C	1:F:396:LEU:CD1	2.79	0.50
1:A:328:ILE:HD11	1:A:407:LEU:HD12	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:347[A]:TYR:CD2	1:H:347[A]:TYR:N	2.78	0.49
1:F:123:TRP:CE3	1:F:162:VAL:HG11	2.47	0.49
1:G:440:ALA:CA	3:G:2521:HOH:O	2.61	0.49
1:F:69:LEU:O	1:F:213:THR:HB	2.12	0.49
1:B:307:LYS:HD3	3:B:2043:HOH:O	2.12	0.49
1:B:347[A]:TYR:H	1:B:347[A]:TYR:HD2	1.54	0.49
1:G:296:LEU:HD12	1:G:530:LEU:HD12	1.91	0.49
1:H:296:LEU:HD12	1:H:347[A]:TYR:CE1	2.46	0.49
1:G:162:VAL:HG23	1:G:162:VAL:O	2.13	0.49
1:E:269:MET:SD	1:E:538:MET:CE	3.00	0.49
1:H:299:TYR:CZ	1:H:439:ARG:HD3	2.47	0.49
1:D:433:GLY:HA2	3:D:3188:HOH:O	2.12	0.49
1:E:428[A]:ASP:HB3	3:E:2659:HOH:O	2.12	0.49
1:D:244:ILE:CD1	1:D:538:MET:HB2	2.43	0.48
1:G:69:LEU:O	1:G:213:THR:HB	2.13	0.48
1:D:47:SER:HB3	3:D:3190:HOH:O	2.09	0.48
1:A:485:GLU:HG3	3:A:3252:HOH:O	2.13	0.48
1:C:488:ARG:NH2	3:C:1595:HOH:O	2.39	0.48
1:F:40:THR:O	1:F:540:ILE:CD1	2.60	0.48
1:H:349:ASP:O	1:H:449:PRO:HD3	2.14	0.48
1:C:123:TRP:CE3	1:C:162:VAL:HG11	2.48	0.48
1:H:309:PRO:HG3	1:H:385:LEU:HD11	1.96	0.48
1:D:467:TYR:CE2	1:D:499:LEU:HD12	2.49	0.48
1:H:301:TYR:HB2	1:H:506:VAL:HB	1.94	0.48
1:A:485:GLU:OE2	1:A:488:ARG:NH1	2.46	0.48
1:D:386:THR:CG2	3:D:2390:HOH:O	2.60	0.48
1:E:460:SER:CB	3:E:2784:HOH:O	2.47	0.48
1:A:69:LEU:O	1:A:213:THR:HB	2.13	0.48
1:B:263:ARG:NH1	1:B:282:LEU:HD23	2.28	0.48
1:G:310:PHE:CZ	1:G:387:ILE:HG21	2.45	0.48
1:H:73:LEU:HD12	1:H:185:LEU:HD13	1.96	0.48
1:H:347[A]:TYR:H	1:H:347[A]:TYR:HD2	1.58	0.48
1:E:275:PRO:HG2	1:E:278:LEU:HB2	1.96	0.47
1:E:323:MET:SD	1:E:328:ILE:CD1	3.03	0.47
1:B:263:ARG:HH11	1:B:282:LEU:HD23	1.78	0.47
1:B:282:LEU:HD22	1:B:516:LEU:HD11	1.96	0.47
1:C:391:TYR:CZ	1:C:420:ASN:HB3	2.49	0.47
1:F:208:PRO:O	3:F:1700:HOH:O	2.20	0.47
1:B:69:LEU:O	1:B:213:THR:HB	2.14	0.47
1:H:512:VAL:CG2	3:H:2459:HOH:O	2.50	0.47
1:G:283:LYS:HD2	3:G:2454:HOH:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:484:ASP:OD1	1:G:486:ALA:N	2.41	0.47
1:H:162:VAL:HG12	1:H:172:VAL:HG13	1.96	0.47
1:A:488:ARG:NH2	3:A:1460:HOH:O	2.48	0.47
1:E:162[A]:VAL:HG23	1:E:162[A]:VAL:O	2.13	0.47
1:F:373:LEU:HD13	3:F:2710:HOH:O	2.14	0.47
1:H:514:ALA:N	3:H:2459:HOH:O	2.48	0.47
3:D:2967:HOH:O	2:L:1:LYS:HD3	2.14	0.47
1:E:261:ARG:HD3	1:E:266:GLU:OE2	2.15	0.47
1:G:279:PHE:HA	1:G:282:LEU:HD12	1.96	0.47
1:E:162[B]:VAL:HG22	3:E:2511:HOH:O	2.13	0.47
1:F:39:GLN:HA	1:F:540:ILE:HD12	1.96	0.47
1:G:307:LYS:HD2	3:G:1324:HOH:O	2.14	0.47
1:B:443:CYS:HB3	3:B:2369:HOH:O	2.14	0.46
1:B:521:VAL:CG1	1:B:538:MET:HE2	2.45	0.46
1:G:440:ALA:O	3:G:2521:HOH:O	2.21	0.46
1:G:117:GLN:HG3	3:G:3228:HOH:O	2.15	0.46
1:H:127:VAL:O	3:H:2702:HOH:O	2.21	0.46
1:F:318:ALA:CB	1:F:374:LEU:HG	2.46	0.46
1:H:530:LEU:N	1:H:530:LEU:HD12	2.30	0.46
1:B:532:ASN:HB3	3:B:1892:HOH:O	2.15	0.46
1:F:73:LEU:C	1:F:74:LEU:HD12	2.35	0.46
1:F:233:SER:N	3:F:2653:HOH:O	2.49	0.46
1:C:349:ASP:O	1:C:449:PRO:HD3	2.15	0.46
1:C:73:LEU:C	1:C:74:LEU:HD12	2.36	0.46
1:G:193:VAL:HG22	3:G:2762:HOH:O	2.14	0.46
1:G:417:LYS:HG3	3:G:3191:HOH:O	2.15	0.46
1:B:395:ASP:O	1:B:399:LYS:HG3	2.16	0.46
1:E:396:LEU:HD13	1:E:400:LEU:HD22	1.96	0.46
1:G:130:ASN:HB3	3:G:3104:HOH:O	2.17	0.45
1:B:340:ALA:HA	1:B:510:TYR:CE2	2.51	0.45
1:H:340:ALA:HA	1:H:510:TYR:CE2	2.50	0.45
1:E:58:GLU:CD	3:E:2832:HOH:O	2.55	0.45
1:E:485:GLU:OE2	1:E:488:ARG:NH1	2.49	0.45
1:C:48:GLU:HG2	3:C:3004:HOH:O	2.16	0.45
1:F:168:HIS:CD2	3:F:3183:HOH:O	2.69	0.45
1:E:305:ASN:HA	3:E:3206:HOH:O	2.15	0.45
1:E:347[B]:TYR:H	1:E:347[B]:TYR:HD2	1.54	0.45
1:C:296:LEU:HD12	1:C:530:LEU:CD1	2.47	0.45
1:D:244:ILE:HD11	1:D:538:MET:HB2	1.99	0.45
1:A:455:THR:HG21	3:A:2523:HOH:O	2.16	0.45
1:B:313:VAL:HB	3:B:2682:HOH:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:ILE:HA	3:C:2419:HOH:O	2.16	0.45
1:E:396:LEU:HD13	1:E:396:LEU:C	2.36	0.45
1:F:168:HIS:HB2	3:F:2576:HOH:O	2.16	0.45
1:A:123:TRP:HE3	1:A:162:VAL:HG11	1.82	0.45
1:H:176:GLU:HB2	1:H:177:PRO:CD	2.47	0.45
1:H:292:VAL:HG13	3:H:2459:HOH:O	2.15	0.45
1:D:331:LYS:HE3	1:D:403:ALA:HB2	1.99	0.44
1:E:124:GLN:N	3:E:2640:HOH:O	2.31	0.44
1:E:439:ARG:HD2	1:E:440:ALA:N	2.32	0.44
1:G:46:GLY:O	3:G:2420:HOH:O	2.20	0.44
1:C:347[A]:TYR:CD2	1:C:347[A]:TYR:N	2.85	0.44
1:A:277:GLU:H	1:A:277:GLU:CD	2.20	0.44
1:G:38:LYS:O	1:G:540:ILE:HD12	2.18	0.44
1:H:179:PRO:HB2	3:H:2497:HOH:O	2.17	0.44
3:D:2967:HOH:O	2:L:1:LYS:CD	2.66	0.44
1:E:165:ILE:HG13	3:E:3172:HOH:O	2.17	0.44
1:F:141:TYR:CE1	1:F:454:ASN:HB3	2.52	0.44
1:F:498:GLN:CD	3:F:2320:HOH:O	2.53	0.44
1:H:128:ASP:HB2	1:H:157:ILE:HG21	1.99	0.44
1:D:517:VAL:HG12	1:D:521:VAL:HB	1.99	0.44
1:B:484:ASP:HB2	3:D:612:HOH:O	2.17	0.44
1:G:468:LYS:HE3	3:G:2222:HOH:O	2.17	0.44
1:H:172:VAL:HG11	1:H:181:PHE:CZ	2.52	0.44
1:F:83:ALA:HB1	1:F:84:PRO:CD	2.48	0.44
1:F:505:ILE:HG22	3:F:2316:HOH:O	2.18	0.44
1:G:521:VAL:HG12	1:G:538:MET:HE2	1.99	0.44
1:G:51:SER:CB	3:G:2800:HOH:O	2.61	0.44
1:H:484:ASP:OD1	1:H:485:GLU:N	2.50	0.44
1:D:168:HIS:ND1	3:D:916:HOH:O	2.29	0.43
1:H:162:VAL:HG21	3:H:2655:HOH:O	2.07	0.43
1:E:297:CYS:HB2	1:E:511:TYR:CG	2.53	0.43
1:G:283:LYS:HG2	3:G:3074:HOH:O	2.18	0.43
1:G:482:VAL:HG21	1:G:488:ARG:HB2	2.00	0.43
1:D:310:PHE:HZ	1:D:387:ILE:HG21	1.82	0.43
1:H:464:THR:OG1	3:H:2711:HOH:O	2.12	0.43
1:A:301:TYR:HB2	1:A:506:VAL:HB	2.01	0.43
1:A:302:GLU:C	3:A:2590:HOH:O	2.51	0.43
1:B:309:PRO:HG3	1:B:385:LEU:HD11	2.00	0.43
1:C:69:LEU:O	1:C:213:THR:HB	2.18	0.43
1:C:456:MET:HG3	1:C:499:LEU:HD21	2.01	0.43
1:D:51:SER:C	3:D:3239:HOH:O	2.57	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:241:LYS:HD3	3:G:2443:HOH:O	2.17	0.43
1:H:216:ALA:CB	3:H:2444:HOH:O	2.24	0.43
1:D:240:ALA:HB1	1:H:235:THR:HG22	1.99	0.43
1:D:501:LYS:HE3	3:D:2700:HOH:O	2.18	0.43
1:E:277:GLU:HG2	3:E:2705:HOH:O	2.18	0.43
1:A:60:VAL:HA	2:I:1:LYS:HD2	2.00	0.43
1:D:345:PRO:HD3	1:D:452:PHE:CZ	2.54	0.43
1:A:269:MET:SD	1:A:538:MET:HE1	2.58	0.43
1:A:321:LEU:HD22	1:A:366:ARG:HG2	2.01	0.43
3:D:2428:HOH:O	2:L:1:LYS:HE3	2.19	0.43
1:F:296:LEU:HD22	1:F:529:PRO:HB2	2.01	0.43
1:A:296:LEU:HD12	1:A:347[A]:TYR:HE1	1.82	0.43
1:C:94:ASP:O	1:C:94:ASP:OD2	2.36	0.43
1:D:49:VAL:CG2	3:D:3239:HOH:O	2.65	0.43
1:G:276:ILE:HG13	1:G:396:LEU:HD23	2.00	0.43
1:C:94:ASP:HB2	3:C:935:HOH:O	2.18	0.43
1:H:39:GLN:HB3	1:H:244:ILE:HA	2.00	0.43
1:A:428[A]:ASP:HB3	3:A:992:HOH:O	2.19	0.43
1:B:280:GLN:HG2	3:B:1749:HOH:O	2.18	0.43
1:E:340:ALA:HA	1:E:510:TYR:CE2	2.54	0.43
1:D:69:LEU:O	1:D:213:THR:HB	2.19	0.42
1:D:269:MET:HG2	1:D:517:VAL:HG13	2.02	0.42
1:F:86:VAL:HG12	1:F:102:LEU:HG	2.01	0.42
1:F:396:LEU:HD13	1:F:396:LEU:O	2.18	0.42
1:B:396:LEU:HD13	1:B:396:LEU:C	2.39	0.42
1:A:69:LEU:HD21	1:A:230:LEU:HD22	2.01	0.42
1:D:297:CYS:HB2	1:D:511:TYR:CG	2.54	0.42
1:E:540:ILE:CD1	3:E:2695:HOH:O	2.67	0.42
1:F:196:ALA:HB3	3:F:2771:HOH:O	2.19	0.42
1:H:439:ARG:HD2	1:H:440:ALA:N	2.35	0.42
1:F:60:VAL:HG22	2:N:1:LYS:HE3	2.01	0.42
1:G:283:LYS:NZ	3:G:1834:HOH:O	2.48	0.42
1:G:432:GLN:NE2	3:G:2354:HOH:O	2.52	0.42
1:A:69:LEU:HA	3:A:2692:HOH:O	2.19	0.42
1:D:207:GLN:HG3	3:D:3088:HOH:O	2.19	0.42
1:E:58:GLU:OE2	3:E:2832:HOH:O	2.22	0.42
1:C:275:PRO:HG2	1:C:278:LEU:HB2	2.02	0.42
1:A:438:ALA:C	3:A:2573:HOH:O	2.58	0.42
1:D:69:LEU:HD21	1:D:230:LEU:HD22	2.01	0.42
1:D:430:ARG:HA	1:D:435:PHE:CE2	2.55	0.42
1:E:427:LEU:HD22	3:E:3109:HOH:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:60:VAL:N	1:H:61:PRO:CD	2.83	0.41
1:B:345:PRO:HD3	1:B:452:PHE:CE1	2.55	0.41
1:E:485:GLU:CD	1:E:488:ARG:NH1	2.73	0.41
1:F:373:LEU:HD21	3:F:1103:HOH:O	2.20	0.41
1:G:296:LEU:HD23	1:G:347:TYR:CE1	2.55	0.41
1:D:324:ASP:OD1	1:D:327:ILE:HD12	2.20	0.41
1:E:391:TYR:CZ	1:E:420:ASN:HB3	2.55	0.41
1:F:288:ASP:OD1	3:F:2868:HOH:O	2.22	0.41
1:F:345:PRO:HG2	3:F:3173:HOH:O	2.19	0.41
1:H:109:SER:N	1:H:213:THR:O	2.51	0.41
1:A:389:LEU:HD13	1:A:437:VAL:HG12	2.02	0.41
1:C:102:LEU:CG	3:C:2541:HOH:O	2.47	0.41
1:D:291:HIS:O	1:D:514:ALA:HA	2.21	0.41
1:G:253:ALA:N	3:G:2420:HOH:O	2.52	0.41
1:C:269:MET:SD	1:C:538:MET:HE3	2.61	0.41
1:D:269:MET:SD	1:D:538:MET:HE1	2.61	0.41
1:E:143:HIS:HB2	3:E:3073:HOH:O	2.20	0.41
1:E:178:VAL:HG23	3:E:3073:HOH:O	2.20	0.41
1:G:299:TYR:CZ	1:G:439:ARG:HD3	2.56	0.41
1:H:423:TRP:CE2	1:H:427:LEU:HD11	2.56	0.41
1:A:259:VAL:O	1:A:263:ARG:HG2	2.20	0.41
1:C:162:VAL:HG12	1:C:172:VAL:HG13	2.03	0.41
1:E:283:LYS:HA	1:E:290:VAL:HG21	2.03	0.41
1:E:423:TRP:CE2	1:E:427:LEU:HD11	2.55	0.41
1:A:309:PRO:HG3	1:A:385:LEU:HD11	2.03	0.41
1:A:352:LYS:NZ	1:E:79:ASP:CG	2.74	0.41
1:E:276:ILE:HD11	1:E:396:LEU:HD22	2.02	0.41
1:E:439:ARG:HB3	3:E:2485:HOH:O	2.20	0.41
1:F:140:GLN:CA	1:F:147:ILE:HD13	2.51	0.41
1:F:209:GLY:N	3:F:2535:HOH:O	2.41	0.41
1:A:39:GLN:HA	1:A:540:ILE:HD13	2.03	0.41
1:H:72:GLY:HA3	3:H:572:HOH:O	2.21	0.41
1:H:276:ILE:HG13	1:H:396:LEU:HD23	2.02	0.41
1:A:328:ILE:HD11	1:A:407:LEU:CD1	2.51	0.40
1:B:372:LYS:HB2	3:B:3193:HOH:O	2.21	0.40
1:F:306:GLN:OE1	1:F:468:LYS:HE2	2.22	0.40
1:G:77:ASP:OD2	1:G:77:ASP:C	2.60	0.40
1:A:521:VAL:CG1	1:A:538:MET:HE2	2.52	0.40
1:D:130:ASN:CG	3:D:2421:HOH:O	2.60	0.40
1:E:323:MET:SD	1:E:328:ILE:HD11	2.61	0.40
1:G:381:ALA:HB2	3:G:2959:HOH:O	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:432:GLN:C	3:C:2446:HOH:O	2.59	0.40
1:G:300:TYR:O	3:G:2521:HOH:O	2.22	0.40
1:G:340:ALA:HA	1:G:510:TYR:CE2	2.56	0.40
1:H:158:THR:HG23	3:H:2593:HOH:O	2.21	0.40
1:B:375:ALA:HB3	3:B:2531:HOH:O	2.20	0.40
1:C:65:ILE:CD1	1:C:228:ILE:HD12	2.51	0.40
1:E:347[A]:TYR:CD2	3:E:3179:HOH:O	2.74	0.40
1:F:135:TYR:CE1	1:F:187:HIS:CE1	3.10	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%)	507 (98%)	9 (2%)	1 (0%)	44	42
1	B	518/524 (99%)	504 (97%)	13 (2%)	1 (0%)	44	42
1	C	517/524 (99%)	502 (97%)	14 (3%)	1 (0%)	44	42
1	D	518/524 (99%)	504 (97%)	13 (2%)	1 (0%)	44	42
1	E	518/524 (99%)	505 (98%)	12 (2%)	1 (0%)	44	42
1	F	516/524 (98%)	501 (97%)	14 (3%)	1 (0%)	44	42
1	G	517/524 (99%)	504 (98%)	12 (2%)	1 (0%)	44	42
1	H	517/524 (99%)	503 (97%)	13 (2%)	1 (0%)	44	42
2	I	1/3 (33%)	1 (100%)	0	0	100	100
2	J	1/3 (33%)	1 (100%)	0	0	100	100
2	K	1/3 (33%)	1 (100%)	0	0	100	100
2	L	1/3 (33%)	1 (100%)	0	0	100	100
2	M	1/3 (33%)	1 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	1/3 (33%)	1 (100%)	0	0	100	100
2	O	1/3 (33%)	1 (100%)	0	0	100	100
2	P	1/3 (33%)	1 (100%)	0	0	100	100
All	All	4146/4216 (98%)	4038 (97%)	100 (2%)	8 (0%)	44	42

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	251	PRO
1	H	251	PRO
1	B	251	PRO
1	D	251	PRO
1	E	251	PRO
1	G	251	PRO
1	C	251	PRO
1	F	251	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	453/458 (99%)	448 (99%)	5 (1%)	70	76
1	B	454/458 (99%)	448 (99%)	6 (1%)	65	71
1	C	453/458 (99%)	448 (99%)	5 (1%)	70	76
1	D	454/458 (99%)	448 (99%)	6 (1%)	65	71
1	E	454/458 (99%)	451 (99%)	3 (1%)	81	86
1	F	452/458 (99%)	445 (98%)	7 (2%)	60	66
1	G	453/458 (99%)	449 (99%)	4 (1%)	75	81
1	H	453/458 (99%)	447 (99%)	6 (1%)	65	71
2	I	2/2 (100%)	1 (50%)	1 (50%)	0	0
2	J	2/2 (100%)	1 (50%)	1 (50%)	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	K	2/2 (100%)	1 (50%)	1 (50%)	0	0
2	L	2/2 (100%)	2 (100%)	0	100	100
2	M	2/2 (100%)	2 (100%)	0	100	100
2	N	2/2 (100%)	2 (100%)	0	100	100
2	O	2/2 (100%)	1 (50%)	1 (50%)	0	0
2	P	2/2 (100%)	2 (100%)	0	100	100
All	All	3642/3680 (99%)	3596 (99%)	46 (1%)	70	71

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	347[A]	TYR
1	A	347[B]	TYR
1	A	369	GLU
1	A	424	LYS
1	A	483	THR
1	B	113	PRO
1	B	347[A]	TYR
1	B	347[B]	TYR
1	B	373	LEU
1	B	418	LEU
1	B	420	ASN
1	C	91	ASP
1	C	277	GLU
1	C	329	VAL
1	C	347[A]	TYR
1	C	347[B]	TYR
1	D	278	LEU
1	D	319	LEU
1	D	347[A]	TYR
1	D	347[B]	TYR
1	D	382	ASP
1	D	405	SER
1	E	163	LYS
1	E	280	GLN
1	E	439	ARG
1	F	91	ASP
1	F	102	LEU
1	F	174	LEU
1	F	176	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	296	LEU
1	F	330	ASN
1	F	484	ASP
1	G	37	GLU
1	G	91	ASP
1	G	331	LYS
1	G	420	ASN
1	H	91	ASP
1	H	277	GLU
1	H	347[A]	TYR
1	H	347[B]	TYR
1	H	349	ASP
1	H	488	ARG
2	I	1	LYS
2	J	1	LYS
2	K	3	GLU
2	O	3	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	HIS
1	B	330	ASN
1	D	466	HIS
1	E	305	ASN
1	G	187	HIS
1	H	124	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	517/524 (98%)	-0.28	2 (0%) 89 88	6, 19, 33, 47	2 (0%)
1	B	517/524 (98%)	-0.15	2 (0%) 89 88	7, 23, 41, 52	4 (0%)
1	C	517/524 (98%)	-0.21	1 (0%) 92 91	8, 21, 33, 43	3 (0%)
1	D	517/524 (98%)	-0.10	5 (0%) 79 78	8, 22, 41, 52	4 (0%)
1	E	517/524 (98%)	-0.15	3 (0%) 85 85	7, 21, 37, 48	4 (0%)
1	F	517/524 (98%)	-0.12	1 (0%) 92 91	10, 23, 37, 44	2 (0%)
1	G	517/524 (98%)	-0.05	2 (0%) 89 88	11, 25, 38, 48	3 (0%)
1	H	516/524 (98%)	0.44	21 (4%) 42 40	16, 32, 57, 69	2 (0%)
2	I	3/3 (100%)	0.07	0 100 100	20, 20, 22, 29	0
2	J	3/3 (100%)	0.16	0 100 100	22, 22, 22, 33	0
2	K	3/3 (100%)	0.14	0 100 100	20, 20, 22, 27	0
2	L	3/3 (100%)	0.99	0 100 100	22, 22, 26, 31	0
2	M	3/3 (100%)	0.22	0 100 100	19, 19, 22, 29	0
2	N	3/3 (100%)	0.02	0 100 100	22, 22, 26, 27	0
2	O	3/3 (100%)	0.09	0 100 100	21, 21, 24, 31	0
2	P	3/3 (100%)	0.54	0 100 100	25, 25, 27, 35	0
All	All	4159/4216 (98%)	-0.08	37 (0%) 81 80	6, 23, 41, 69	24 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	484	ASP	3.8
1	E	347[A]	TYR	3.4
1	H	347[A]	TYR	3.3
1	H	201	PHE	3.1
1	H	198	ILE	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	280	GLN	2.8
1	H	178	VAL	2.8
1	H	200	LYS	2.7
1	D	280	GLN	2.6
1	D	277	GLU	2.5
1	C	94	ASP	2.5
1	G	175	SER	2.4
1	D	485	GLU	2.4
1	G	364	GLU	2.4
1	D	347[A]	TYR	2.4
1	H	27	ALA	2.3
1	B	347[A]	TYR	2.3
1	A	277	GLU	2.3
1	H	203	GLU	2.3
1	H	180	TYR	2.2
1	H	112	THR	2.2
1	H	208	PRO	2.2
1	H	146	GLY	2.2
1	H	90	TRP	2.2
1	H	486	ALA	2.2
1	H	170	LEU	2.1
1	B	381	ALA	2.1
1	E	209	GLY	2.1
1	H	132	ALA	2.1
1	A	347[A]	TYR	2.1
1	H	93	LYS	2.1
1	H	95	ALA	2.1
1	H	102	LEU	2.1
1	D	330	ASN	2.0
1	H	97	VAL	2.0
1	H	143	HIS	2.0
1	E	278	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides 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.