



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:56 PM UTC

PDB ID : 2W80 / pdb_00002w80
Title : Structure of a complex between Neisseria meningitidis factor H binding protein and CCPs 6-7 of human complement factor H
Authors : Schneider, M.C.; Prosser, B.E.; Caesar, J.J.E.; Kugelberg, E.; Li, S.; Zhang, Q.; Quoraishi, S.; Lovett, J.E.; Deane, J.E.; Sim, R.B.; Roversi, P.; Johnson, S.; Tang, C.M.; Lea, S.M.
Deposited on : 2009-01-08
Resolution : 2.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

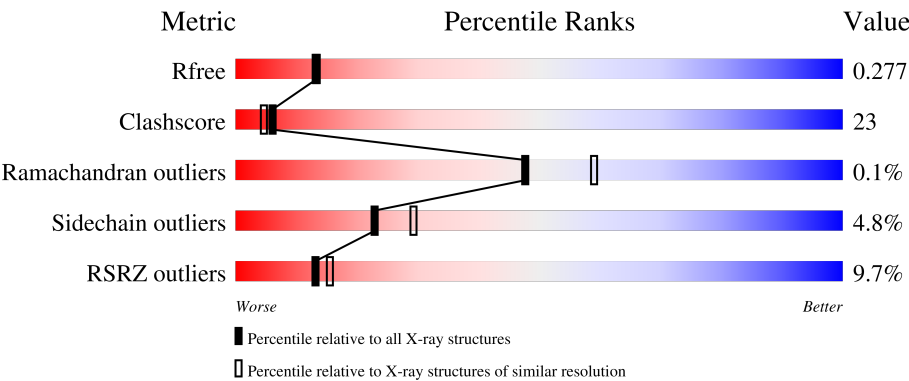
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	123	7% 65% 29% 6%
1	B	123	7% 65% 33% .
1	E	123	6% 65% 33% .
1	G	123	11% 59% 37% .
2	C	253	10% 53% 40% . .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	253	6% 60% 34%
2	F	253	11% 58% 36%
2	H	253	14% 57% 36%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11942 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 COMPLEMENT FACTOR H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	123	Total	C	N	O	S	0	1	0
			1005	643	171	181	10			
1	B	123	Total	C	N	O	S	0	0	0
			999	639	171	179	10			
1	E	123	Total	C	N	O	S	0	0	0
			999	639	171	179	10			
1	G	123	Total	C	N	O	S	0	0	0
			999	639	171	179	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	402	HIS	TYR	variant	UNP P08603
B	402	HIS	TYR	variant	UNP P08603
E	402	HIS	TYR	variant	UNP P08603
G	402	HIS	TYR	variant	UNP P08603

- Molecule 2 is a protein called FACTOR H BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	243	Total	C	N	O	S	0	1	0
			1844	1145	331	367	1			
2	D	244	Total	C	N	O	S	0	2	0
			1861	1155	335	370	1			
2	F	244	Total	C	N	O	S	0	3	0
			1866	1158	335	372	1			
2	H	244	Total	C	N	O	S	0	2	0
			1861	1155	335	370	1			

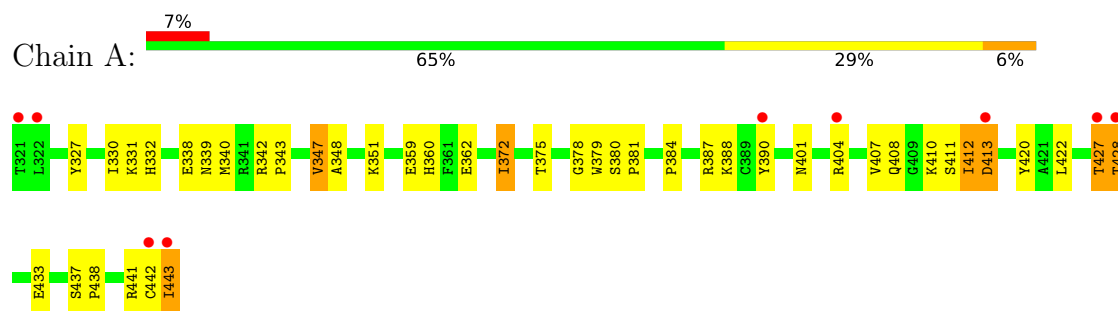
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	64	Total O 64 64	0	0
3	B	43	Total O 43 43	0	0
3	C	92	Total O 92 92	0	0
3	D	104	Total O 104 104	0	0
3	E	39	Total O 39 39	0	0
3	F	77	Total O 77 77	0	0
3	G	33	Total O 33 33	0	0
3	H	56	Total O 56 56	0	0

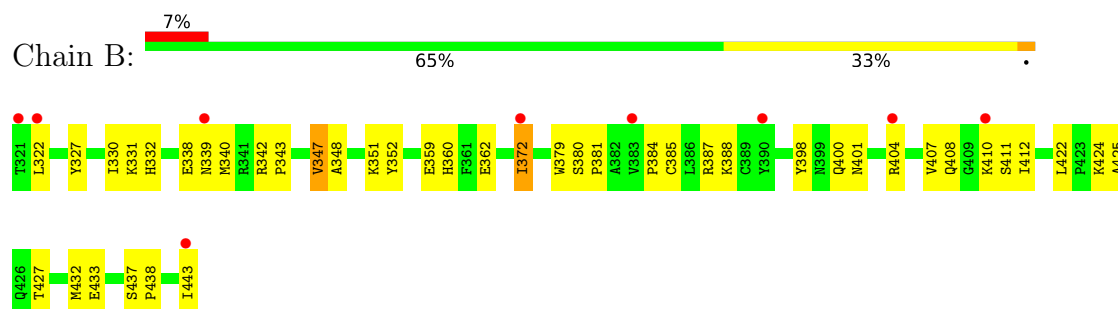
3 Residue-property plots

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.

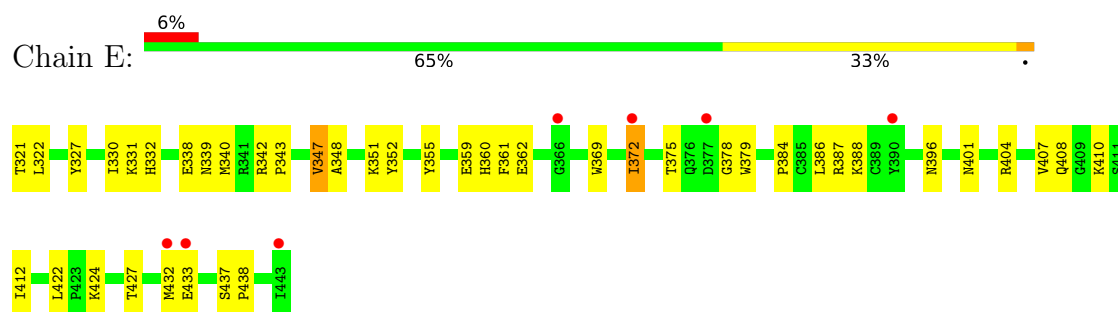
• Molecule 1: COMPLEMENT FACTOR H



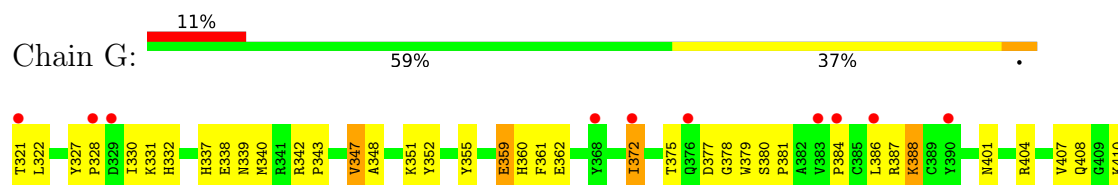
• Molecule 1: COMPLEMENT FACTOR H

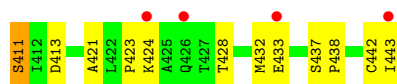


• Molecule 1: COMPLEMENT FACTOR H

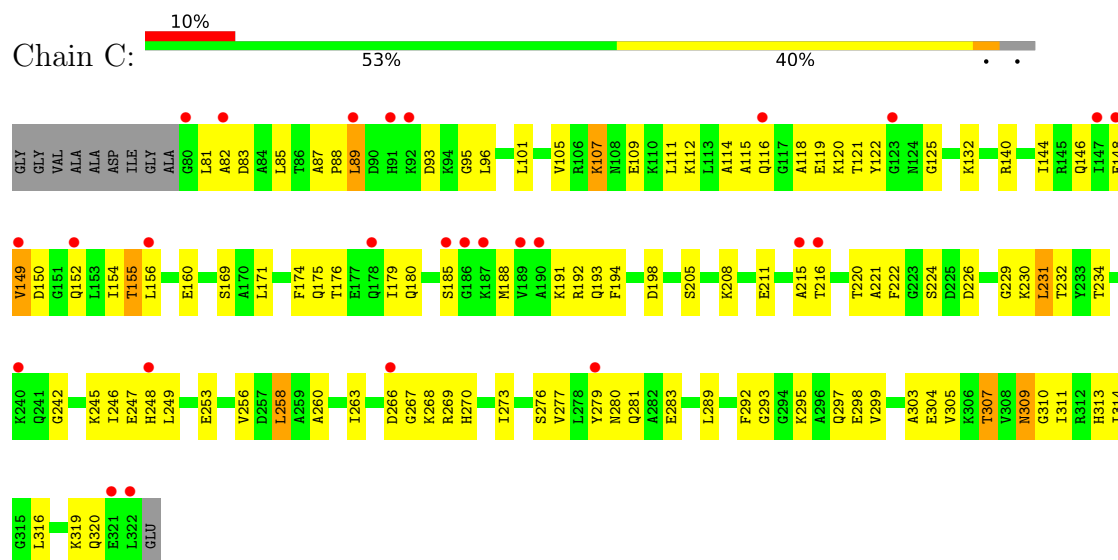


• Molecule 1: COMPLEMENT FACTOR H

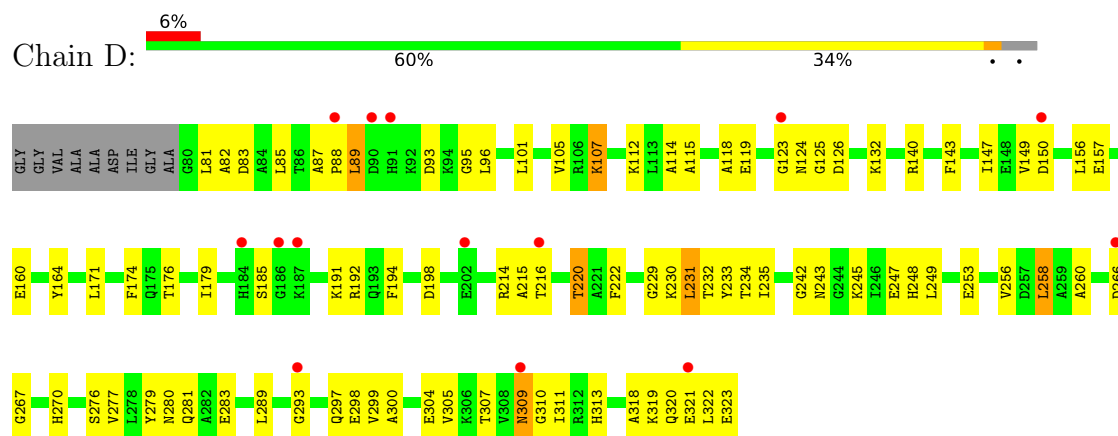




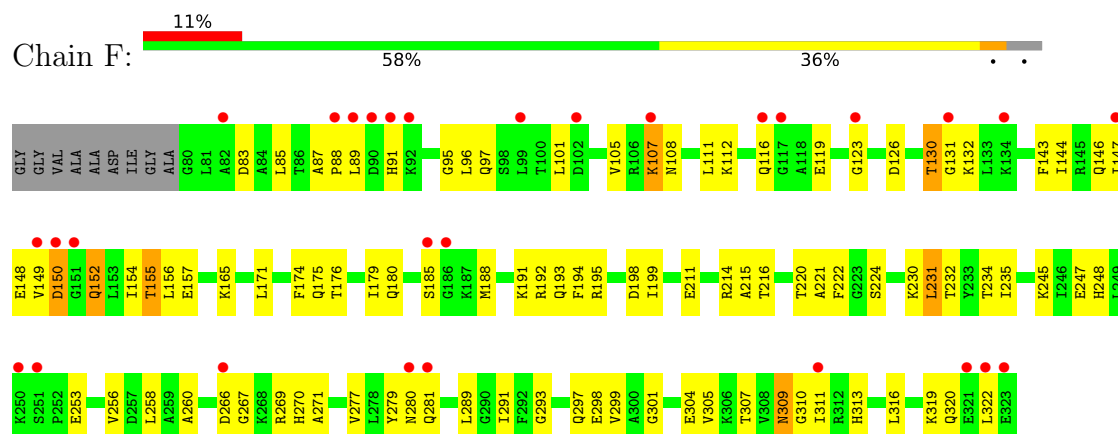
- Molecule 2: FACTOR H BINDING PROTEIN



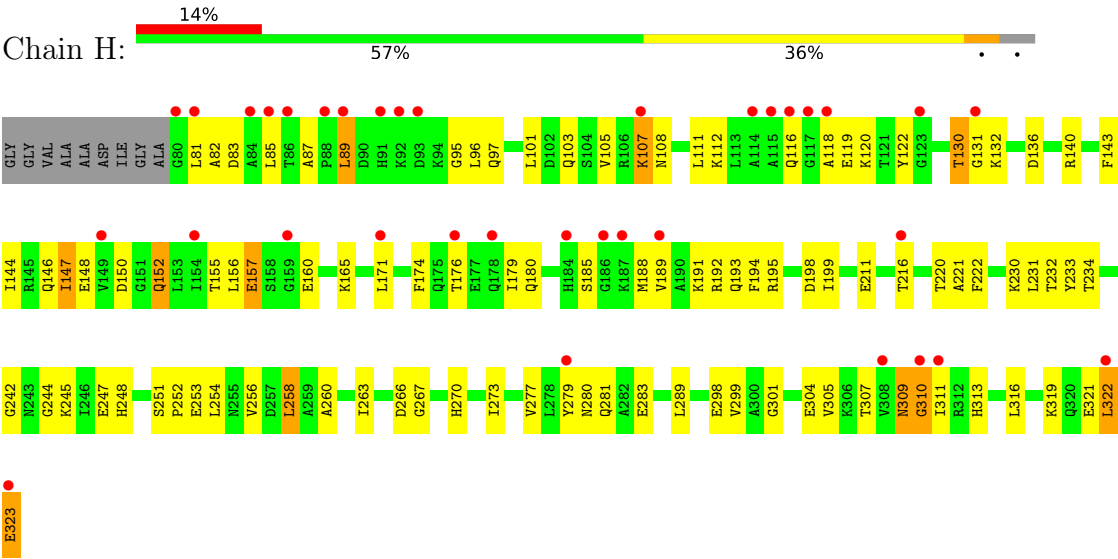
- Molecule 2: FACTOR H BINDING PROTEIN



- Molecule 2: FACTOR H BINDING PROTEIN



● Molecule 2: FACTOR H BINDING PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	48.70Å 93.85Å 99.72Å 80.07° 80.18° 84.81°	Depositor
Resolution (Å)	95.00 – 2.35 95.00 – 2.35	Depositor EDS
% Data completeness (in resolution range)	91.8 (95.00-2.35) 92.0 (95.00-2.35)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 2.14Å)	Xtriage
Refinement program		Depositor
R, R_{free}	0.233 , 0.263 0.237 , 0.277	Depositor DCC
R_{free} test set	3938 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	33.5	Xtriage
Anisotropy	0.420	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11942	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.56	0/1048	0.86	1/1429 (0.1%)
1	B	0.50	0/1039	0.84	2/1417 (0.1%)
1	E	0.46	0/1039	0.83	2/1417 (0.1%)
1	G	0.47	0/1039	0.84	1/1417 (0.1%)
2	C	0.51	0/1872	0.89	4/2511 (0.2%)
2	D	0.51	0/1892	0.89	3/2537 (0.1%)
2	F	0.51	0/1900	0.89	5/2548 (0.2%)
2	H	0.52	0/1892	0.90	4/2537 (0.2%)
All	All	0.51	0/11721	0.87	22/15813 (0.1%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	132	LYS	N-CA-C	-8.01	103.22	113.16
2	C	125	GLY	N-CA-C	-7.40	105.30	114.92
2	C	267	GLY	N-CA-C	-6.60	106.17	114.16
2	H	267	GLY	N-CA-C	-6.53	106.26	114.16
2	D	309	ASN	N-CA-C	6.50	124.16	113.89
2	F	130	THR	N-CA-C	-6.37	102.31	110.53
2	F	132	LYS	N-CA-C	-6.28	105.60	113.20
2	C	309	ASN	N-CA-C	5.93	123.26	113.89
2	D	267	GLY	N-CA-C	-5.88	107.37	114.66
2	H	309	ASN	N-CA-C	5.86	123.14	113.89
2	F	309	ASN	N-CA-C	5.83	123.09	113.89
1	E	422	LEU	CA-C-N	-5.68	114.76	120.21
1	E	422	LEU	C-N-CA	-5.68	114.76	120.21
1	B	422	LEU	CA-C-N	-5.63	114.45	120.03
1	B	422	LEU	C-N-CA	-5.63	114.45	120.03
2	D	125	GLY	N-CA-C	-5.53	107.73	114.92
2	C	149	VAL	CB-CA-C	-5.49	102.94	110.96
1	G	424	LYS	CA-CB-CG	-5.43	103.25	114.10
2	F	150	ASP	N-CA-C	-5.24	99.63	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	130	THR	N-CA-C	-5.24	103.97	110.41
1	A	412	ILE	N-CA-C	5.10	116.06	108.46
2	F	267	GLY	N-CA-C	-5.07	106.58	113.37

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	1005	0	921	42	0
1	B	999	0	915	37	0
1	E	999	0	915	34	0
1	G	999	0	915	45	0
2	C	1844	0	1833	96	0
2	D	1861	0	1852	76	0
2	F	1866	0	1856	87	0
2	H	1861	0	1852	98	0
3	A	64	0	0	2	0
3	B	43	0	0	1	0
3	C	92	0	0	1	0
3	D	104	0	0	4	0
3	E	39	0	0	3	0
3	F	77	0	0	3	0
3	G	33	0	0	3	0
3	H	56	0	0	3	0
All	All	11942	0	11059	508	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 23.

All (508) 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)
2:C:89:LEU:H	2:C:89:LEU:HD13	1.10	1.12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:149:VAL:O	2:C:152:GLN:HG2	1.47	1.12
2:H:147:ILE:HG12	2:H:156:LEU:HD11	1.29	1.09
2:H:322:LEU:C	2:H:323:GLU:HG2	1.79	1.04
2:H:89:LEU:H	2:H:89:LEU:HD13	1.13	1.02
2:D:105:VAL:O	2:D:124:ASN:ND2	1.96	0.99
1:A:420:TYR:CD1	1:A:443:ILE:HG12	1.99	0.98
2:C:231:LEU:HD12	2:C:232:THR:N	1.82	0.95
2:D:89:LEU:HD13	2:D:89:LEU:H	1.31	0.94
2:H:147:ILE:HG12	2:H:156:LEU:CD1	1.99	0.92
2:H:171:LEU:HD11	2:H:222:PHE:HZ	1.33	0.92
2:C:231:LEU:HD22	2:C:316:LEU:HD22	1.52	0.91
1:B:407:VAL:HG12	1:B:410:LYS:HE3	1.52	0.91
2:H:231:LEU:HD12	2:H:232:THR:N	1.86	0.90
2:C:171:LEU:HD11	2:C:222:PHE:HZ	1.37	0.90
2:F:231:LEU:HD22	2:F:316:LEU:HD22	1.51	0.90
2:H:152:GLN:HA	2:H:152:GLN:NE2	1.84	0.90
2:C:230:LYS:HD3	2:C:248:HIS:ND1	1.87	0.90
2:F:171:LEU:HD11	2:F:222:PHE:CZ	2.06	0.90
1:A:442:CYS:O	1:A:443:ILE:HG13	1.72	0.90
2:C:289:LEU:HD13	2:C:299:VAL:HG11	1.56	0.88
2:F:171:LEU:HD11	2:F:222:PHE:HZ	1.36	0.88
1:B:407:VAL:HG12	1:B:410:LYS:CE	2.03	0.87
2:H:171:LEU:HD11	2:H:222:PHE:CZ	2.09	0.87
2:F:231:LEU:HD12	2:F:232:THR:N	1.89	0.86
2:F:215:ALA:HB1	2:F:320:GLN:OE1	1.75	0.86
2:C:89:LEU:HD13	2:C:89:LEU:N	1.90	0.86
1:A:420:TYR:HD1	1:A:443:ILE:HG12	1.43	0.83
2:H:322:LEU:O	2:H:323:GLU:HG2	1.77	0.83
2:D:230:LYS:HD3	2:D:248:HIS:ND1	1.93	0.83
2:C:171:LEU:HD11	2:C:222:PHE:CZ	2.14	0.82
2:H:89:LEU:H	2:H:89:LEU:CD1	1.93	0.82
1:B:407:VAL:H	1:B:410:LYS:HD2	1.44	0.81
2:F:289:LEU:HD13	2:F:299:VAL:HG11	1.63	0.81
2:C:89:LEU:H	2:C:89:LEU:CD1	1.89	0.81
2:H:231:LEU:HD22	2:H:316:LEU:HD22	1.63	0.81
2:H:253:GLU:OE1	2:H:307:THR:HB	1.81	0.80
1:A:410:LYS:HD2	1:A:411:SER:H	1.47	0.80
2:D:89:LEU:H	2:D:89:LEU:CD1	1.96	0.79
2:F:253:GLU:OE1	2:F:307:THR:HB	1.83	0.79
2:D:231:LEU:HD13	2:D:232:THR:N	1.98	0.78
2:D:89:LEU:HD13	2:D:89:LEU:N	1.98	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:131:GLY:HA2	2:H:165:LYS:NZ	1.99	0.77
2:D:253:GLU:OE1	2:D:307:THR:HB	1.85	0.77
2:C:149:VAL:O	2:C:152:GLN:CG	2.28	0.77
2:C:215:ALA:HB1	2:C:320:GLN:OE1	1.86	0.76
2:H:230:LYS:HD3	2:H:248:HIS:ND1	1.98	0.76
1:A:410:LYS:HD2	1:A:411:SER:N	2.01	0.76
2:H:231:LEU:HD12	2:H:232:THR:H	1.50	0.76
1:B:407:VAL:N	1:B:410:LYS:HD2	2.00	0.75
2:H:309:ASN:H	2:H:310:GLY:HA2	1.49	0.75
2:H:309:ASN:N	2:H:310:GLY:HA2	2.02	0.75
1:G:423:PRO:HA	1:G:443:ILE:HD11	1.68	0.75
1:G:372:ILE:HG13	1:G:379:TRP:CE3	2.21	0.75
2:C:107:LYS:O	2:C:107:LYS:HD3	1.88	0.74
2:H:116:GLN:HA	3:H:2008:HOH:O	1.86	0.74
2:F:230:LYS:HD3	2:F:248:HIS:ND1	2.02	0.74
2:F:309:ASN:N	2:F:310:GLY:HA2	2.02	0.73
2:D:231:LEU:HD13	2:D:231:LEU:C	2.13	0.73
2:C:309:ASN:N	2:C:310:GLY:HA2	2.04	0.73
2:H:289:LEU:HD22	2:H:299:VAL:HG12	1.70	0.73
2:D:289:LEU:HD13	2:D:299:VAL:HG11	1.69	0.72
2:F:107:LYS:O	2:F:107:LYS:HD3	1.90	0.72
2:D:164:TYR:CE2	2:D:220:THR:HG21	2.25	0.72
2:H:107:LYS:O	2:H:107:LYS:HD3	1.90	0.72
2:H:156:LEU:HD23	2:H:180:GLN:NE2	2.05	0.71
2:D:171:LEU:HD11	2:D:222:PHE:CZ	2.24	0.71
2:H:89:LEU:HD13	2:H:89:LEU:N	1.98	0.71
2:C:253:GLU:OE1	2:C:307:THR:HB	1.90	0.70
2:F:123:GLY:HA3	2:F:126:ASP:OD2	1.90	0.70
2:F:107:LYS:HD3	2:F:107:LYS:C	2.15	0.70
2:C:146:GLN:HG2	2:C:155:THR:HA	1.73	0.69
1:E:372:ILE:HG13	1:E:379:TRP:CE3	2.28	0.69
2:F:309:ASN:H	2:F:310:GLY:HA2	1.56	0.69
2:H:146:GLN:HG2	2:H:155:THR:HA	1.74	0.69
2:H:289:LEU:HD13	2:H:299:VAL:HG11	1.75	0.69
2:D:215:ALA:HB1	2:D:320:GLN:OE1	1.92	0.68
1:E:332:HIS:NE2	1:E:433:GLU:OE2	2.18	0.68
2:F:256:VAL:HG21	2:F:277:VAL:HG13	1.73	0.68
1:A:359[A]:GLU:H	1:A:359[A]:GLU:CD	2.02	0.68
2:F:171:LEU:CD1	2:F:222:PHE:HZ	2.06	0.67
2:D:107:LYS:HD3	2:D:107:LYS:C	2.17	0.67
2:C:289:LEU:HD22	2:C:299:VAL:HG12	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:321:THR:N	3:E:2001:HOH:O	2.27	0.67
2:H:174:PHE:HB3	3:H:2021:HOH:O	1.93	0.67
1:B:372:ILE:HG12	1:B:379:TRP:CE3	2.29	0.67
2:F:256:VAL:HG21	2:F:277:VAL:CG1	2.25	0.67
2:F:289:LEU:HD22	2:F:299:VAL:HG12	1.76	0.67
2:H:107:LYS:HD3	2:H:107:LYS:C	2.19	0.66
2:C:107:LYS:HD3	2:C:107:LYS:C	2.19	0.66
1:A:428:THR:HG22	3:A:2056:HOH:O	1.95	0.66
2:D:309:ASN:N	2:D:310:GLY:HA2	2.10	0.66
2:D:107:LYS:HD3	2:D:107:LYS:O	1.96	0.66
2:C:93:ASP:OD2	2:C:132:LYS:HE2	1.97	0.65
2:D:171:LEU:HD11	2:D:222:PHE:HZ	1.61	0.65
2:H:256:VAL:HG12	2:H:279:TYR:HB2	1.79	0.65
2:H:322:LEU:C	2:H:323:GLU:CG	2.59	0.65
2:D:304:GLU:HG2	2:D:313:HIS:CD2	2.32	0.65
1:A:442:CYS:O	1:A:443:ILE:CG1	2.44	0.65
2:C:107:LYS:HA	2:C:107:LYS:HE3	1.79	0.65
1:A:372:ILE:HG12	1:A:379:TRP:CE3	2.31	0.64
2:H:107:LYS:HA	2:H:107:LYS:HE3	1.78	0.64
2:H:180:GLN:OE1	2:H:185:SER:HA	1.98	0.64
2:C:156:LEU:HD23	2:C:180:GLN:NE2	2.12	0.64
2:F:156:LEU:HD23	2:F:180:GLN:NE2	2.12	0.64
2:F:149:VAL:O	2:F:150:ASP:HB2	1.97	0.64
1:A:347:VAL:CG1	1:A:351:LYS:HB2	2.28	0.63
1:G:342:ARG:HB3	1:G:343:PRO:HD3	1.79	0.63
2:H:304:GLU:HG2	2:H:313:HIS:CD2	2.34	0.63
2:D:309:ASN:H	2:D:310:GLY:HA2	1.64	0.62
2:C:309:ASN:H	2:C:310:GLY:HA2	1.63	0.62
1:A:420:TYR:CE1	1:A:443:ILE:HG12	2.35	0.62
1:B:342:ARG:HB3	1:B:343:PRO:HD3	1.80	0.62
2:C:216:THR:HG22	2:C:234:THR:OG1	1.99	0.62
1:E:362:GLU:OE1	1:E:388:LYS:NZ	2.33	0.62
1:A:362:GLU:OE1	1:A:388:LYS:NZ	2.32	0.62
1:A:327:TYR:OH	1:A:338:GLU:HG3	1.98	0.62
2:C:144:ILE:HG22	2:C:146:GLN:HG3	1.82	0.62
2:D:93:ASP:OD2	2:D:132:LYS:HE2	1.98	0.62
2:F:179:ILE:HD13	2:F:191:LYS:HD3	1.80	0.62
2:H:83:ASP:OD1	2:H:87:ALA:HB2	1.98	0.62
2:C:231:LEU:HD12	2:C:232:THR:H	1.61	0.61
2:D:289:LEU:HD22	2:D:299:VAL:HG12	1.80	0.61
2:D:95:GLY:HA2	2:D:96:LEU:C	2.25	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:CYS:C	1:A:443:ILE:HG13	2.23	0.61
1:E:355:TYR:CD2	1:E:372:ILE:HG23	2.35	0.61
2:D:107:LYS:HE3	2:D:107:LYS:HA	1.82	0.61
2:F:107:LYS:HE3	2:F:107:LYS:HA	1.83	0.61
2:F:143:PHE:HE1	2:F:157:GLU:HG2	1.65	0.61
1:G:355:TYR:CD2	1:G:372:ILE:CG2	2.84	0.61
1:B:387:ARG:HG2	1:B:432:MET:O	2.00	0.60
2:H:256:VAL:HG21	2:H:277:VAL:HG13	1.82	0.60
2:F:256:VAL:CG2	2:F:277:VAL:HG13	2.30	0.60
1:B:332:HIS:NE2	1:B:433:GLU:OE2	2.25	0.60
2:F:180:GLN:OE1	2:F:185:SER:HA	2.02	0.59
1:A:420:TYR:HD1	1:A:443:ILE:CG1	2.12	0.59
1:B:327:TYR:OH	1:B:338:GLU:HG3	2.02	0.59
1:B:359:GLU:O	1:B:360:HIS:HB2	2.01	0.59
2:D:179:ILE:HD13	2:D:191:LYS:HD3	1.83	0.59
2:F:147:ILE:CG2	2:F:156:LEU:HD11	2.33	0.59
2:C:171:LEU:CD1	2:C:222:PHE:HZ	2.14	0.59
1:E:342:ARG:HB3	1:E:343:PRO:HD3	1.84	0.59
2:D:123:GLY:O	2:D:126:ASP:HB2	2.03	0.58
1:G:330:ILE:HG23	1:G:384:PRO:CG	2.33	0.58
2:H:131:GLY:HA2	2:H:165:LYS:HZ2	1.67	0.58
2:D:171:LEU:CD1	2:D:222:PHE:HZ	2.16	0.58
2:F:149:VAL:HB	2:F:154:ILE:HD13	1.85	0.58
2:H:289:LEU:HD22	2:H:299:VAL:CG1	2.33	0.58
2:D:143:PHE:CE1	2:D:157:GLU:HG2	2.38	0.58
1:A:347:VAL:HG11	1:A:351:LYS:HB2	1.85	0.58
2:F:131:GLY:HA2	2:F:165:LYS:NZ	2.18	0.58
1:G:442:CYS:HB2	3:G:2025:HOH:O	2.04	0.58
2:D:112:LYS:HE2	2:D:119:GLU:OE2	2.04	0.58
2:H:176:THR:O	2:H:192:ARG:HA	2.04	0.58
2:D:83:ASP:OD1	2:D:87:ALA:HB2	2.03	0.58
2:C:256:VAL:HG12	2:C:279:TYR:HB2	1.86	0.58
1:E:401:ASN:HA	1:E:404:ARG:HD3	1.85	0.58
1:G:359:GLU:O	1:G:360:HIS:HB2	2.04	0.57
2:D:140:ARG:HB3	2:D:160:GLU:OE2	2.04	0.57
2:H:216:THR:HG22	2:H:234:THR:OG1	2.05	0.57
2:F:112:LYS:HE2	2:F:119:GLU:OE2	2.04	0.57
1:B:372:ILE:HG12	1:B:379:TRP:HE3	1.69	0.57
2:C:95:GLY:HA2	2:C:96:LEU:C	2.29	0.57
1:E:347:VAL:CG1	1:E:351:LYS:HB2	2.34	0.57
1:A:330:ILE:HG23	1:A:384:PRO:HG2	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:VAL:CG1	1:B:351:LYS:HB2	2.34	0.57
1:E:327:TYR:OH	1:E:338:GLU:HG3	2.04	0.57
1:E:407:VAL:HG22	1:E:408:GLN:N	2.19	0.57
1:G:423:PRO:CA	1:G:443:ILE:HD11	2.34	0.57
1:G:327:TYR:OH	1:G:338:GLU:HG3	2.04	0.57
2:F:148:GLU:HA	2:F:152:GLN:O	2.04	0.56
2:H:140:ARG:HD3	2:H:160:GLU:OE2	2.05	0.56
1:E:355:TYR:CD2	1:E:372:ILE:CG2	2.88	0.56
1:G:355:TYR:CD2	1:G:372:ILE:HG22	2.40	0.56
2:F:89:LEU:HA	3:F:2013:HOH:O	2.05	0.56
2:H:95:GLY:HA2	2:H:96:LEU:C	2.31	0.56
2:H:179:ILE:HD13	2:H:191:LYS:HD3	1.86	0.56
2:H:171:LEU:CD1	2:H:222:PHE:HZ	2.13	0.56
2:H:256:VAL:HG21	2:H:277:VAL:CG1	2.36	0.56
2:D:143:PHE:HE1	2:D:157:GLU:HG2	1.70	0.56
1:G:408:GLN:NE2	1:G:433:GLU:HB2	2.21	0.56
2:H:152:GLN:NE2	2:H:152:GLN:CA	2.65	0.56
2:C:83:ASP:OD1	2:C:87:ALA:HB2	2.05	0.55
2:D:231:LEU:C	2:D:231:LEU:CD1	2.78	0.55
2:C:263:ILE:HG12	2:C:273:ILE:HG12	1.88	0.55
1:G:347:VAL:CG1	1:G:351:LYS:HB2	2.36	0.55
1:B:443:ILE:C	1:B:443:ILE:HD12	2.31	0.55
2:F:101:LEU:HA	2:F:198:ASP:OD2	2.06	0.55
1:A:372:ILE:HG12	1:A:379:TRP:HE3	1.69	0.55
1:A:332:HIS:NE2	1:A:433:GLU:OE2	2.26	0.55
1:E:359:GLU:O	1:E:360:HIS:HB2	2.05	0.55
2:F:143:PHE:CE1	2:F:157:GLU:HG2	2.41	0.55
1:G:359:GLU:OE1	2:H:108:ASN:HB2	2.06	0.55
2:C:231:LEU:HD12	2:C:231:LEU:C	2.28	0.55
1:A:342:ARG:HB3	1:A:343:PRO:HD3	1.89	0.55
2:D:256:VAL:HG12	2:D:279:TYR:HB2	1.89	0.55
1:G:332:HIS:NE2	1:G:433:GLU:OE2	2.37	0.55
2:C:298:GLU:HG2	2:C:319:LYS:CB	2.37	0.54
2:D:147:ILE:HD12	2:D:149:VAL:HG23	1.88	0.54
1:A:420:TYR:CD1	1:A:443:ILE:CG1	2.81	0.54
2:C:149:VAL:N	2:C:152:GLN:O	2.34	0.54
1:G:331:LYS:HB3	3:G:2005:HOH:O	2.08	0.54
2:C:256:VAL:HG21	2:C:277:VAL:CG1	2.38	0.54
2:C:220:THR:HG22	2:C:221:ALA:N	2.22	0.54
2:H:280:ASN:O	2:H:281:GLN:HB2	2.07	0.54
1:A:401:ASN:HA	1:A:404:ARG:HD3	1.88	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:322:LEU:HD23	3:D:2097:HOH:O	2.07	0.54
2:D:112:LYS:HZ3	2:D:119:GLU:HG3	1.72	0.54
2:D:280:ASN:O	2:D:281:GLN:HB2	2.07	0.54
2:D:101:LEU:HA	2:D:198:ASP:OD2	2.08	0.53
1:G:421:ALA:O	1:G:443:ILE:HG13	2.07	0.53
2:D:289:LEU:HD22	2:D:299:VAL:CG1	2.37	0.53
2:C:246:ILE:HD11	2:C:316:LEU:HD21	1.90	0.53
2:F:245:LYS:HE3	2:F:247:GLU:OE2	2.08	0.53
2:C:180:GLN:OE1	2:C:185:SER:HA	2.08	0.53
2:F:112:LYS:HZ3	2:F:119:GLU:HG3	1.73	0.53
2:D:300:ALA:CA	3:D:2088:HOH:O	2.57	0.53
2:F:91:HIS:HA	3:F:2003:HOH:O	2.08	0.53
2:H:147:ILE:CG1	2:H:156:LEU:HD11	2.20	0.53
1:B:424:LYS:O	1:B:425:ALA:HB3	2.07	0.53
2:C:231:LEU:CD2	2:C:316:LEU:HD22	2.31	0.53
2:D:245:LYS:HE3	2:D:247:GLU:OE2	2.09	0.53
1:B:339:ASN:OD1	1:B:340:MET:N	2.42	0.53
2:C:112:LYS:HE2	2:C:119:GLU:OE2	2.09	0.52
2:C:289:LEU:HB3	2:C:299:VAL:HG13	1.91	0.52
1:A:330:ILE:HG23	1:A:384:PRO:CG	2.39	0.52
1:B:362:GLU:OE1	1:B:388:LYS:NZ	2.42	0.52
1:G:339:ASN:OD1	1:G:340:MET:N	2.43	0.52
2:C:140:ARG:HB3	2:C:160:GLU:OE2	2.09	0.52
1:G:338:GLU:OE2	1:G:342:ARG:NH2	2.28	0.52
1:B:330:ILE:HG23	1:B:384:PRO:HG2	1.91	0.52
2:H:155:THR:HG22	2:H:188:MET:SD	2.50	0.52
2:H:256:VAL:CG2	2:H:277:VAL:HG13	2.40	0.52
1:E:387:ARG:HG2	1:E:432:MET:O	2.10	0.52
2:F:266:ASP:CB	2:F:270:HIS:H	2.22	0.52
1:B:407:VAL:HG22	1:B:408:GLN:N	2.25	0.51
2:C:268:LYS:O	2:C:269:ARG:HB2	2.10	0.51
2:C:289:LEU:HD13	2:C:299:VAL:CG1	2.35	0.51
1:E:339:ASN:OD1	1:E:340:MET:N	2.43	0.51
2:F:280:ASN:O	2:F:281:GLN:HB2	2.08	0.51
1:G:407:VAL:HG22	1:G:408:GLN:N	2.25	0.51
2:H:143:PHE:HE1	2:H:157:GLU:HG2	1.75	0.51
2:F:116:GLN:HG3	2:F:116:GLN:O	2.11	0.51
1:E:359:GLU:OE1	2:F:108:ASN:HB2	2.10	0.51
1:E:347:VAL:HG11	1:E:351:LYS:HB2	1.91	0.51
1:G:387:ARG:HG2	1:G:432:MET:O	2.11	0.51
2:D:83:ASP:HB2	3:D:2002:HOH:O	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:140:ARG:HD3	2:D:160:GLU:OE2	2.10	0.51
2:F:231:LEU:HD12	2:F:231:LEU:C	2.33	0.51
2:H:140:ARG:HB3	2:H:160:GLU:OE2	2.11	0.51
2:H:245:LYS:HE3	2:H:247:GLU:OE2	2.10	0.51
2:D:147:ILE:HG12	2:D:156:LEU:HD11	1.92	0.51
2:C:149:VAL:HG21	2:C:154:ILE:HD12	1.92	0.50
2:D:88:PRO:O	2:D:89:LEU:C	2.54	0.50
2:H:298:GLU:HG2	2:H:319:LYS:CB	2.41	0.50
1:G:330:ILE:HG23	1:G:384:PRO:HG2	1.92	0.50
2:C:280:ASN:O	2:C:281:GLN:HB2	2.11	0.50
1:B:322:LEU:N	1:B:322:LEU:HD12	2.27	0.50
2:F:147:ILE:HG21	2:F:156:LEU:HD11	1.94	0.50
2:H:101:LEU:HA	2:H:198:ASP:OD2	2.11	0.50
1:G:362:GLU:OE1	1:G:388:LYS:NZ	2.40	0.50
2:H:289:LEU:HB3	2:H:299:VAL:HG13	1.93	0.50
2:F:131:GLY:HA2	2:F:165:LYS:HZ2	1.77	0.50
2:H:195[B]:ARG:HA	2:H:313:HIS:ND1	2.26	0.50
2:D:289:LEU:HB3	2:D:299:VAL:HG13	1.92	0.50
2:H:220:THR:CG2	2:H:221:ALA:N	2.75	0.50
1:B:347:VAL:HG11	1:B:351:LYS:HB2	1.93	0.50
2:H:195[A]:ARG:HA	2:H:313:HIS:ND1	2.26	0.50
1:A:412:ILE:O	1:A:428:THR:HB	2.12	0.49
1:G:322:LEU:N	1:G:322:LEU:HD12	2.27	0.49
2:D:149:VAL:O	2:D:150:ASP:HB2	2.12	0.49
2:D:298:GLU:HG2	2:D:319:LYS:CB	2.42	0.49
2:H:258:LEU:N	2:H:258:LEU:HD12	2.27	0.49
1:B:347:VAL:HG13	1:B:348:ALA:N	2.27	0.49
2:C:116:GLN:O	2:C:116:GLN:HG3	2.12	0.49
2:C:149:VAL:O	2:C:152:GLN:OE1	2.30	0.49
2:D:214:ARG:HA	2:D:235:ILE:O	2.12	0.49
2:F:95:GLY:HA2	2:F:96:LEU:C	2.36	0.49
1:G:347:VAL:HG11	1:G:351:LYS:HB2	1.94	0.49
2:F:155:THR:HG22	2:F:188:MET:SD	2.52	0.49
1:A:412:ILE:CG2	1:A:413:ASP:N	2.75	0.49
2:F:231:LEU:CD2	2:F:316:LEU:HD22	2.35	0.49
1:G:355:TYR:CE2	1:G:372:ILE:HG22	2.48	0.49
1:G:347:VAL:CG1	1:G:348:ALA:N	2.75	0.49
2:F:298:GLU:HG2	2:F:319:LYS:CB	2.42	0.49
2:F:176:THR:O	2:F:192:ARG:HA	2.13	0.49
2:F:289:LEU:HD22	2:F:299:VAL:CG1	2.42	0.49
2:D:298:GLU:HG2	2:D:319:LYS:HB3	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:147:ILE:O	2:F:154:ILE:N	2.40	0.49
1:G:410:LYS:HG3	1:G:411:SER:N	2.26	0.49
2:H:81:LEU:N	2:H:81:LEU:HD23	2.28	0.49
2:H:112:LYS:HE2	2:H:119:GLU:OE2	2.13	0.49
2:H:199:ILE:HD13	2:H:301:GLY:HA2	1.95	0.49
2:F:260:ALA:HB1	3:F:2047:HOH:O	2.13	0.48
1:B:330:ILE:HG23	1:B:384:PRO:CG	2.42	0.48
2:C:155:THR:HG22	2:C:188:MET:SD	2.53	0.48
1:E:338:GLU:OE2	1:E:342:ARG:NH2	2.31	0.48
1:G:442:CYS:C	1:G:443:ILE:HG23	2.39	0.48
1:G:401:ASN:HA	1:G:404:ARG:HD2	1.94	0.48
2:C:101:LEU:HA	2:C:198:ASP:OD2	2.14	0.48
2:C:140:ARG:HD3	2:C:160:GLU:OE2	2.14	0.48
1:E:437:SER:HA	1:E:438:PRO:HA	1.64	0.48
2:F:105:VAL:HG22	2:F:111:LEU:HB2	1.94	0.48
2:F:266:ASP:HB2	2:F:270:HIS:H	1.79	0.48
2:C:179:ILE:HD13	2:C:191:LYS:HD3	1.96	0.48
2:C:229:GLY:HA3	2:C:249:LEU:CD2	2.44	0.48
2:F:199:ILE:HD13	2:F:301:GLY:HA2	1.95	0.48
1:B:437:SER:HA	1:B:438:PRO:HA	1.64	0.48
1:A:407:VAL:HG22	1:A:408:GLN:N	2.29	0.47
2:C:295:LYS:HB2	2:C:297:GLN:NE2	2.29	0.47
1:E:369:TRP:CE2	2:F:195[B]:ARG:HD3	2.49	0.47
1:E:424:LYS:O	1:E:424:LYS:HG2	2.14	0.47
2:H:242:GLY:O	2:H:260:ALA:HA	2.14	0.47
2:H:258:LEU:N	2:H:258:LEU:CD1	2.77	0.47
2:H:307:THR:OG1	2:H:310:GLY:O	2.28	0.47
2:C:191:LYS:HE2	2:C:193:GLN:OE1	2.15	0.47
2:F:216:THR:HG22	2:F:234:THR:OG1	2.14	0.47
2:C:304:GLU:HG2	2:C:313:HIS:CD2	2.49	0.47
1:E:347:VAL:CG1	1:E:348:ALA:N	2.78	0.47
2:C:152:GLN:CG	2:C:152:GLN:O	2.60	0.47
2:D:82:ALA:HA	2:D:118:ALA:HB3	1.97	0.47
2:D:123:GLY:HA3	2:D:126:ASP:OD2	2.15	0.47
1:E:396:ASN:HB2	3:E:2029:HOH:O	2.14	0.47
2:H:220:THR:HG22	2:H:221:ALA:N	2.30	0.47
2:C:220:THR:CG2	2:C:221:ALA:N	2.77	0.47
2:C:226:ASP:HA	3:C:2060:HOH:O	2.14	0.47
1:E:401:ASN:HA	1:E:404:ARG:CD	2.45	0.47
1:G:377:ASP:HB2	3:G:2019:HOH:O	2.14	0.47
1:A:351:LYS:NZ	2:D:276:SER:HB3	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:242:GLY:O	2:C:260:ALA:HA	2.14	0.46
2:F:289:LEU:HB3	2:F:299:VAL:HG13	1.96	0.46
2:D:176:THR:O	2:D:192:ARG:HA	2.15	0.46
2:C:266:ASP:CB	2:C:270:HIS:H	2.28	0.46
2:D:107:LYS:HA	2:D:107:LYS:CE	2.39	0.46
1:A:387:ARG:HD3	1:A:433:GLU:O	2.15	0.46
2:H:105:VAL:HG22	2:H:111:LEU:HB2	1.98	0.46
2:C:81:LEU:C	2:C:83:ASP:N	2.73	0.46
2:F:191:LYS:HE2	2:F:193:GLN:OE1	2.16	0.46
1:A:387:ARG:HG3	1:A:388:LYS:N	2.30	0.46
1:B:432:MET:HG3	1:B:437:SER:HB2	1.97	0.46
2:C:293:GLY:HA3	2:C:297:GLN:OE1	2.16	0.46
2:D:256:VAL:HG21	2:D:277:VAL:CG1	2.45	0.46
2:H:116:GLN:HG3	2:H:116:GLN:O	2.16	0.46
1:B:385:CYS:HB2	3:B:2005:HOH:O	2.16	0.46
1:E:347:VAL:HG13	1:E:348:ALA:N	2.31	0.46
2:H:112:LYS:O	2:H:143:PHE:HA	2.16	0.46
1:A:339:ASN:OD1	1:A:340:MET:N	2.49	0.45
2:C:107:LYS:HA	2:C:107:LYS:CE	2.41	0.45
2:H:305:VAL:O	2:H:311:ILE:HA	2.17	0.45
2:D:112:LYS:HE2	3:D:2014:HOH:O	2.16	0.45
1:E:361:PHE:HA	1:E:386:LEU:O	2.16	0.45
2:F:97:GLN:O	2:F:130:THR:O	2.35	0.45
2:H:144:ILE:HG22	2:H:146:GLN:HG3	1.98	0.45
1:A:331:LYS:O	1:A:332:HIS:HB2	2.16	0.45
2:C:148:GLU:HA	2:C:152:GLN:O	2.17	0.45
2:F:156:LEU:CD2	2:F:180:GLN:NE2	2.80	0.45
2:F:175:GLN:NE2	2:F:224:SER:OG	2.43	0.45
1:G:355:TYR:CD2	1:G:372:ILE:HG23	2.51	0.45
2:H:231:LEU:HD12	2:H:231:LEU:C	2.36	0.45
2:D:231:LEU:HD13	2:D:232:THR:CA	2.47	0.45
2:F:258:LEU:CD1	2:F:258:LEU:N	2.80	0.45
2:C:82:ALA:HA	2:C:118:ALA:HB3	1.99	0.45
2:C:256:VAL:HG21	2:C:277:VAL:HG11	1.98	0.45
1:E:330:ILE:HG23	1:E:384:PRO:HG2	1.98	0.45
1:E:372:ILE:HG13	1:E:379:TRP:CZ3	2.52	0.45
1:G:432:MET:HG3	1:G:437:SER:HB2	1.98	0.45
2:H:143:PHE:HE1	2:H:157:GLU:CG	2.30	0.45
1:A:437:SER:HA	1:A:438:PRO:HA	1.82	0.45
2:C:105:VAL:HG13	2:C:109:GLU:HG3	1.98	0.45
2:F:195[B]:ARG:HA	2:F:313:HIS:ND1	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:VAL:CG1	1:B:348:ALA:N	2.80	0.45
1:G:331:LYS:O	1:G:332:HIS:HB2	2.16	0.45
2:H:156:LEU:CD2	2:H:180:GLN:NE2	2.76	0.45
2:H:194:PHE:HB3	3:H:2024:HOH:O	2.15	0.45
1:B:380:SER:HA	1:B:381:PRO:C	2.41	0.44
2:H:82:ALA:HA	2:H:118:ALA:HB3	1.99	0.44
1:E:331:LYS:O	1:E:332:HIS:HB2	2.17	0.44
1:E:410:LYS:HE3	3:E:2032:HOH:O	2.16	0.44
2:F:305:VAL:O	2:F:311:ILE:HA	2.18	0.44
2:H:97:GLN:O	2:H:130:THR:O	2.35	0.44
1:B:407:VAL:HG12	1:B:410:LYS:NZ	2.33	0.44
1:E:330:ILE:HG23	1:E:384:PRO:CG	2.47	0.44
1:A:442:CYS:HB3	3:A:2037:HOH:O	2.18	0.44
2:C:307:THR:HG23	2:C:310:GLY:O	2.17	0.44
2:F:293:GLY:HA3	2:F:297:GLN:OE1	2.17	0.44
1:G:352:TYR:CE1	2:H:311:ILE:HD13	2.52	0.44
2:C:303:ALA:HB3	2:C:314:ILE:HB	1.99	0.44
2:D:229:GLY:HA3	2:D:249:LEU:CD2	2.48	0.44
1:E:375:THR:OG1	1:E:378:GLY:O	2.33	0.44
2:F:256:VAL:HG12	2:F:279:TYR:HB2	1.99	0.44
2:H:266:ASP:HB2	2:H:270:HIS:H	1.83	0.44
1:A:427:THR:HG23	1:A:428:THR:HG23	1.99	0.44
2:C:150:ASP:C	2:C:152:GLN:H	2.24	0.44
2:D:293:GLY:HA3	2:D:297:GLN:OE1	2.18	0.44
2:F:195[A]:ARG:HA	2:F:313:HIS:ND1	2.32	0.44
1:G:337:HIS:CE1	2:H:103:GLN:HE22	2.36	0.44
1:A:422:LEU:HD23	1:A:441:ARG:O	2.17	0.44
2:C:105:VAL:HG22	2:C:111:LEU:HB2	2.00	0.44
2:F:107:LYS:HA	2:F:107:LYS:CE	2.46	0.44
1:G:321:THR:C	1:G:322:LEU:HD12	2.42	0.44
1:G:407:VAL:HG22	1:G:408:GLN:H	1.83	0.44
1:A:380:SER:HA	1:A:381:PRO:C	2.42	0.44
2:F:144:ILE:HG22	2:F:146:GLN:HG3	1.99	0.44
2:C:245:LYS:HE3	2:C:247:GLU:OE2	2.18	0.43
2:F:231:LEU:HD12	2:F:232:THR:H	1.75	0.43
2:F:304:GLU:HG2	2:F:313:HIS:CD2	2.53	0.43
2:F:147:ILE:HG23	2:F:156:LEU:CD1	2.48	0.43
2:H:251:SER:HB3	2:H:254:LEU:HG	2.00	0.43
2:C:112:LYS:HZ3	2:C:119:GLU:HG3	1.83	0.43
2:C:258:LEU:N	2:C:258:LEU:CD1	2.80	0.43
1:B:398:TYR:HB3	1:B:400:GLN:OE1	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:TYR:CD1	1:A:390:TYR:N	2.86	0.43
2:C:88:PRO:O	2:C:89:LEU:C	2.60	0.43
2:D:164:TYR:CE2	2:D:220:THR:CG2	2.96	0.43
2:F:149:VAL:HB	2:F:154:ILE:CD1	2.48	0.43
2:F:220:THR:HG22	2:F:221:ALA:N	2.32	0.43
2:D:256:VAL:HG21	2:D:277:VAL:HG13	2.01	0.43
2:D:258:LEU:N	2:D:258:LEU:CD1	2.80	0.43
2:D:305:VAL:O	2:D:311:ILE:HA	2.19	0.43
2:C:156:LEU:HD23	2:C:180:GLN:HE22	1.84	0.43
2:D:185:SER:O	2:D:185:SER:OG	2.33	0.43
2:F:214:ARG:HA	2:F:235:ILE:O	2.18	0.43
2:C:149:VAL:O	2:C:152:GLN:CD	2.61	0.43
2:C:307:THR:O	2:C:310:GLY:HA2	2.18	0.43
1:E:407:VAL:HG22	1:E:408:GLN:H	1.83	0.43
2:H:103:GLN:HB2	2:H:198:ASP:OD1	2.19	0.43
2:H:191:LYS:HE2	2:H:193:GLN:OE1	2.19	0.43
2:F:289:LEU:HD13	2:F:299:VAL:CG1	2.42	0.43
1:E:352:TYR:CD1	1:E:352:TYR:C	2.97	0.42
2:F:146:GLN:HG2	2:F:155:THR:HA	2.00	0.42
2:H:148:GLU:HG3	2:H:150:ASP:O	2.19	0.42
1:A:412:ILE:HG22	1:A:413:ASP:N	2.34	0.42
1:B:331:LYS:O	1:B:332:HIS:HB2	2.19	0.42
1:G:328:PRO:HG3	1:G:372:ILE:HD11	2.01	0.42
2:H:233:TYR:HD1	2:H:244:GLY:HA3	1.83	0.42
2:D:266:ASP:HB2	2:D:270:HIS:H	1.85	0.42
1:G:413:ASP:OD1	1:G:428:THR:HG23	2.19	0.42
2:C:298:GLU:HG2	2:C:319:LYS:HB3	2.01	0.42
2:D:216:THR:HG22	2:D:234:THR:OG1	2.19	0.42
2:F:88:PRO:O	2:F:89:LEU:C	2.60	0.42
2:H:107:LYS:HA	2:H:107:LYS:CE	2.45	0.42
2:H:131:GLY:HA2	2:H:165:LYS:CE	2.50	0.42
1:B:432:MET:HG3	1:B:437:SER:CB	2.49	0.42
2:C:266:ASP:HB2	2:C:270:HIS:H	1.85	0.42
2:D:231:LEU:HD11	2:D:233:TYR:HB2	2.01	0.42
2:D:266:ASP:CB	2:D:270:HIS:H	2.32	0.42
2:F:271:ALA:HB1	2:F:291:ILE:HD12	2.01	0.42
2:F:112:LYS:O	2:F:143:PHE:HA	2.19	0.42
2:H:263:ILE:HG12	2:H:273:ILE:HG12	2.01	0.42
2:D:242:GLY:O	2:D:260:ALA:HA	2.20	0.42
1:G:372:ILE:HG13	1:G:379:TRP:HE3	1.76	0.42
2:H:298:GLU:HG2	2:H:319:LYS:HB3	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:VAL:CG1	1:A:348:ALA:N	2.82	0.42
1:B:401:ASN:O	1:B:404:ARG:HB2	2.20	0.42
1:B:407:VAL:H	1:B:410:LYS:NZ	2.18	0.42
2:C:175:GLN:NE2	2:C:224:SER:OG	2.48	0.42
2:F:256:VAL:HG21	2:F:277:VAL:HG11	2.01	0.42
2:H:266:ASP:CB	2:H:270:HIS:H	2.33	0.42
1:B:352:TYR:CD1	1:B:352:TYR:C	2.98	0.42
2:H:81:LEU:C	2:H:83:ASP:N	2.76	0.42
2:H:112:LYS:HZ3	2:H:119:GLU:HG3	1.84	0.42
2:H:120:LYS:HD3	2:H:122:TYR:CZ	2.55	0.42
1:B:407:VAL:HG12	1:B:410:LYS:CD	2.49	0.41
2:H:83:ASP:OD1	2:H:87:ALA:CB	2.66	0.41
2:H:174:PHE:O	2:H:194:PHE:HA	2.20	0.41
2:C:83:ASP:OD1	2:C:87:ALA:CB	2.69	0.41
2:C:120:LYS:HG2	2:C:121:THR:N	2.35	0.41
2:C:176:THR:O	2:C:192:ARG:HA	2.21	0.41
2:C:305:VAL:O	2:C:311:ILE:HA	2.20	0.41
1:G:347:VAL:HG13	1:G:348:ALA:N	2.35	0.41
2:D:230:LYS:HD3	2:D:248:HIS:CE1	2.54	0.41
2:F:220:THR:CG2	2:F:221:ALA:N	2.84	0.41
2:C:205:SER:HB3	2:C:208:LYS:HB2	2.03	0.41
2:C:289:LEU:HD22	2:C:299:VAL:CG1	2.47	0.41
2:H:143:PHE:CD1	2:H:143:PHE:C	2.98	0.41
1:A:375:THR:OG1	1:A:378:GLY:O	2.32	0.41
2:D:114:ALA:O	2:D:115:ALA:HB2	2.19	0.41
2:F:180:GLN:OE1	2:F:185:SER:HB2	2.21	0.41
2:F:269:ARG:NH1	2:F:269:ARG:HG2	2.36	0.41
2:C:114:ALA:O	2:C:115:ALA:HB2	2.21	0.41
2:C:120:LYS:HD3	2:C:122:TYR:OH	2.21	0.41
2:C:185:SER:O	2:C:185:SER:OG	2.37	0.41
2:C:289:LEU:HB3	2:C:299:VAL:CG1	2.51	0.41
2:D:81:LEU:C	2:D:83:ASP:N	2.75	0.41
2:D:231:LEU:HD12	2:D:318:ALA:HB2	2.02	0.41
2:F:87:ALA:HA	2:F:88:PRO:HD3	1.95	0.41
1:G:361:PHE:HA	1:G:386:LEU:O	2.21	0.41
2:C:298:GLU:HG2	2:C:319:LYS:HB2	2.02	0.41
2:D:143:PHE:CD1	2:D:143:PHE:C	2.99	0.41
2:H:251:SER:HA	2:H:252:PRO:HD3	1.93	0.41
1:B:372:ILE:HG21	1:B:372:ILE:HD13	1.83	0.40
2:C:169:SER:HB3	2:C:292:PHE:CG	2.56	0.40
2:D:174:PHE:O	2:D:194:PHE:HA	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:322:LEU:N	1:E:322:LEU:HD12	2.36	0.40
2:F:174:PHE:O	2:F:194:PHE:HA	2.21	0.40
1:G:380:SER:HA	1:G:381:PRO:C	2.46	0.40
1:G:437:SER:HA	1:G:438:PRO:HA	1.64	0.40
1:B:351:LYS:HZ1	2:C:276:SER:HB3	1.86	0.40
2:F:258:LEU:N	2:F:258:LEU:HD12	2.36	0.40
2:H:136:ASP:OD2	2:H:319:LYS:NZ	2.46	0.40
2:H:289:LEU:HD13	2:H:299:VAL:CG1	2.48	0.40
1:A:372:ILE:HD11	1:A:379:TRP:HB3	2.03	0.40
1:G:375:THR:OG1	1:G:378:GLY:O	2.34	0.40
2:C:152:GLN:HG2	2:C:152:GLN:O	2.21	0.40
2:C:174:PHE:O	2:C:194:PHE:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	122/123 (99%)	115 (94%)	7 (6%)	0	100	100
1	B	121/123 (98%)	114 (94%)	7 (6%)	0	100	100
1	E	121/123 (98%)	115 (95%)	6 (5%)	0	100	100
1	G	121/123 (98%)	114 (94%)	7 (6%)	0	100	100
2	C	242/253 (96%)	227 (94%)	15 (6%)	0	100	100
2	D	244/253 (96%)	231 (95%)	13 (5%)	0	100	100
2	F	245/253 (97%)	228 (93%)	16 (6%)	1 (0%)	30	34
2	H	244/253 (96%)	227 (93%)	16 (7%)	1 (0%)	30	34
All	All	1460/1504 (97%)	1371 (94%)	87 (6%)	2 (0%)	48	59

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	152	GLN
2	H	310	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	109/108 (101%)	103 (94%)	6 (6%)	19	24
1	B	108/108 (100%)	103 (95%)	5 (5%)	24	31
1	E	108/108 (100%)	104 (96%)	4 (4%)	30	40
1	G	108/108 (100%)	103 (95%)	5 (5%)	24	31
2	C	191/194 (98%)	182 (95%)	9 (5%)	23	30
2	D	193/194 (100%)	184 (95%)	9 (5%)	23	30
2	F	194/194 (100%)	188 (97%)	6 (3%)	35	47
2	H	193/194 (100%)	180 (93%)	13 (7%)	15	17
All	All	1204/1208 (100%)	1147 (95%)	57 (5%)	23	30

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	347	VAL
1	A	372	ILE
1	A	413	ASP
1	A	427	THR
1	A	428	THR
1	A	443	ILE
1	B	347	VAL
1	B	372	ILE
1	B	411	SER
1	B	412	ILE
1	B	427	THR
2	C	85	LEU
2	C	89	LEU
2	C	107	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	155	THR
2	C	211	GLU
2	C	231	LEU
2	C	258	LEU
2	C	283	GLU
2	C	307	THR
2	D	85	LEU
2	D	89	LEU
2	D	107	LYS
2	D	220	THR
2	D	231	LEU
2	D	258	LEU
2	D	283	GLU
2	D	321	GLU
2	D	323	GLU
1	E	347	VAL
1	E	372	ILE
1	E	412	ILE
1	E	427	THR
2	F	85	LEU
2	F	107	LYS
2	F	155	THR
2	F	211	GLU
2	F	231	LEU
2	F	322	LEU
1	G	347	VAL
1	G	359	GLU
1	G	372	ILE
1	G	388	LYS
1	G	411	SER
2	H	85	LEU
2	H	89	LEU
2	H	107	LYS
2	H	147	ILE
2	H	152	GLN
2	H	157	GLU
2	H	189	VAL
2	H	211	GLU
2	H	258	LEU
2	H	283	GLU
2	H	321	GLU
2	H	322	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	323	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	417	HIS
1	B	396	ASN
1	B	417	HIS
2	C	135	ASN
2	C	146	GLN
2	C	175	GLN
2	D	129	ASN
2	D	166	GLN
2	D	184	HIS
2	D	193	GLN
1	E	396	ASN
2	F	162	GLN
2	F	175	GLN
1	G	417	HIS
2	H	108	ASN
2	H	152	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 [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	123/123 (100%)	0.63	9 (7%)	21 24	22, 33, 49, 66	3 (2%)
1	B	123/123 (100%)	0.79	9 (7%)	21 24	29, 40, 54, 66	2 (1%)
1	E	123/123 (100%)	0.85	7 (5%)	29 34	30, 41, 54, 68	2 (1%)
1	G	123/123 (100%)	1.00	14 (11%)	10 11	33, 44, 58, 71	1 (0%)
2	C	243/253 (96%)	0.80	26 (10%)	11 13	20, 38, 55, 68	1 (0%)
2	D	244/253 (96%)	0.58	14 (5%)	29 34	14, 34, 51, 64	2 (0%)
2	F	244/253 (96%)	0.82	29 (11%)	9 10	17, 39, 60, 75	3 (1%)
2	H	244/253 (96%)	1.09	35 (14%)	6 7	20, 43, 62, 73	2 (0%)
All	All	1467/1504 (97%)	0.82	143 (9%)	13 15	14, 39, 57, 75	16 (1%)

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	443	ILE	6.3
2	H	118	ALA	4.7
2	C	89	LEU	4.0
2	C	321	GLU	4.0
2	H	323	GLU	3.8
1	A	404	ARG	3.8
1	E	390	TYR	3.8
1	G	443	ILE	3.7
2	H	86	THR	3.6
2	C	189	VAL	3.5
2	F	91	HIS	3.4
1	E	443	ILE	3.4
1	B	390	TYR	3.4
2	D	321	GLU	3.3
2	C	123	GLY	3.2
2	H	186	GLY	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	89	LEU	3.2
2	C	149	VAL	3.2
2	F	280	ASN	3.2
2	H	89	LEU	3.2
2	F	90	ASP	3.1
2	H	149	VAL	3.1
2	H	322	LEU	3.1
2	F	92	LYS	3.1
2	H	91	HIS	3.1
1	A	390	TYR	3.0
2	F	131	GLY	3.0
1	B	410	LYS	3.0
1	B	443	ILE	3.0
2	F	311	ILE	3.0
2	H	310	GLY	3.0
2	F	150	ASP	3.0
1	G	372	ILE	3.0
2	H	80	GLY	3.0
2	F	323	GLU	3.0
1	E	372	ILE	2.9
2	C	266	ASP	2.9
2	C	82	ALA	2.9
2	C	147	ILE	2.9
2	F	117	GLY	2.8
1	G	368	TYR	2.8
2	C	91	HIS	2.8
2	H	116	GLN	2.8
2	F	107	LYS	2.8
2	H	311	ILE	2.8
2	H	184	HIS	2.8
2	F	116	GLN	2.8
2	H	88	PRO	2.8
2	D	293	GLY	2.7
2	H	92	LYS	2.7
2	C	156	LEU	2.7
2	D	91	HIS	2.7
1	G	383	VAL	2.7
2	H	216	THR	2.7
2	C	190	ALA	2.7
2	H	114	ALA	2.6
2	C	216	THR	2.6
1	B	404	ARG	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	428	THR	2.6
2	F	151	GLY	2.6
2	H	117	GLY	2.6
2	C	152	GLN	2.6
1	A	442	CYS	2.6
2	H	115	ALA	2.6
1	A	427	THR	2.6
1	G	384	PRO	2.6
2	H	187	LYS	2.6
2	C	80	GLY	2.6
2	F	149	VAL	2.6
2	F	266	ASP	2.5
2	C	187	LYS	2.5
1	A	321	THR	2.5
1	A	413	ASP	2.5
2	F	321	GLU	2.4
2	H	85	LEU	2.4
2	H	171	LEU	2.4
2	C	178	GLN	2.4
2	H	123	GLY	2.4
1	E	433	GLU	2.4
1	A	322	LEU	2.4
2	D	266	ASP	2.4
2	F	147	ILE	2.4
1	G	386	LEU	2.4
2	H	81	LEU	2.4
1	G	321	THR	2.3
2	H	189	VAL	2.3
2	F	186	GLY	2.3
1	B	372	ILE	2.3
1	G	329	ASP	2.3
2	D	123	GLY	2.3
2	H	159	GLY	2.3
1	E	432	MET	2.3
2	C	215	ALA	2.3
1	G	426	GLN	2.3
2	H	84	ALA	2.3
2	F	251	SER	2.3
1	G	376	GLN	2.3
2	H	154	ILE	2.3
1	G	433	GLU	2.2
2	F	281	GLN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	176	THR	2.2
2	D	309	ASN	2.2
2	F	102	ASP	2.2
2	C	185	SER	2.2
2	C	279	TYR	2.2
1	E	366	GLY	2.2
2	F	250	LYS	2.2
1	B	321	THR	2.2
1	G	390	TYR	2.2
2	H	308	VAL	2.2
2	D	216	THR	2.2
2	H	279	TYR	2.1
2	D	150	ASP	2.1
2	H	178	GLN	2.1
1	B	339	ASN	2.1
1	B	383	VAL	2.1
2	C	116	GLN	2.1
2	D	88	PRO	2.1
2	C	186	GLY	2.1
2	F	123	GLY	2.1
2	F	82	ALA	2.1
2	C	92	LYS	2.1
2	D	202	GLU	2.1
2	F	322	LEU	2.1
2	C	248	HIS	2.1
2	F	185	SER	2.1
1	B	322	LEU	2.1
2	F	88	PRO	2.1
2	D	186	GLY	2.1
2	H	131	GLY	2.1
1	G	424	LYS	2.0
2	D	187	LYS	2.0
2	H	107	LYS	2.0
2	C	148	GLU	2.0
1	E	377	ASP	2.0
2	C	322	LEU	2.0
2	C	240	LYS	2.0
2	F	134	LYS	2.0
2	D	184	HIS	2.0
2	D	90	ASP	2.0
2	F	99	LEU	2.0
2	H	93	ASP	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	328	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.