



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 11, 2024 – 03:17 am GMT

PDB ID : 8PWU
Title : PfRH5 bound to monoclonal antibody MAD10-255
Authors : Farrell, B.; Higgins, M.K.
Deposited on : 2023-07-21
Resolution : 3.15 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)	:	1.13
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)	:	2.40

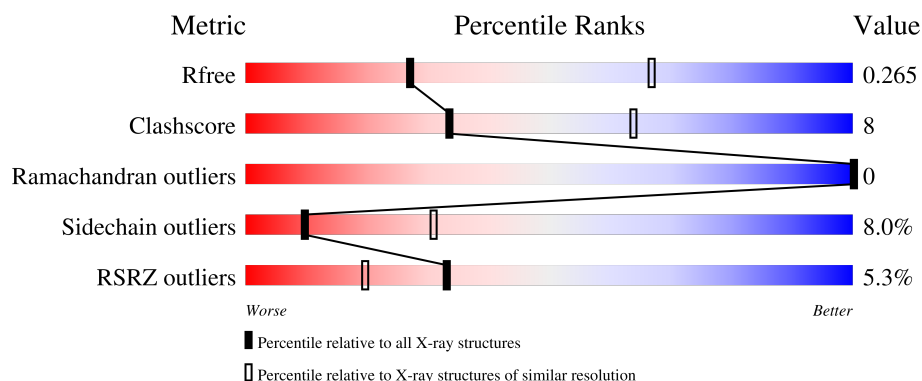
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	2149 (3.18-3.10)
Clashscore	180529	2290 (3.18-3.10)
Ramachandran outliers	177936	2178 (3.18-3.10)
Sidechain outliers	177891	2178 (3.18-3.10)
RSRZ outliers	164620	2149 (3.18-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	338	<div> <div>3%</div> <div>68% 17% 15%</div> </div>
1	C	338	<div> <div>5%</div> <div>66% 17% 15%</div> </div>
1	E	338	<div> <div>4%</div> <div>67% 17% 15%</div> </div>
1	G	338	<div> <div>0%</div> <div>70% 14% 15%</div> </div>
1	I	338	<div> <div>7%</div> <div>67% 16% 15%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K	338	<div><div></div><div>9%</div><div>69%</div><div>15%</div><div>•</div><div>15%</div></div>
2	B	250	<div><div></div><div>3%</div><div>63%</div><div>23%</div><div>•</div><div>11%</div></div>
2	D	250	<div><div></div><div>4%</div><div>67%</div><div>21%</div><div>•</div><div>10%</div></div>
2	F	250	<div><div></div><div>2%</div><div>65%</div><div>24%</div><div>•</div><div>10%</div></div>
2	H	250	<div><div></div><div>2%</div><div>64%</div><div>23%</div><div>•</div><div>10%</div></div>
2	J	250	<div><div></div><div>11%</div><div>66%</div><div>20%</div><div>•</div><div>11%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23363 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 Reticulocyte-binding protein homolog 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	0	0
			2443	1575	411	442	15			
1	C	288	Total	C	N	O	S	0	0	0
			2443	1575	411	442	15			
1	E	287	Total	C	N	O	S	0	0	0
			2435	1571	409	440	15			
1	G	286	Total	C	N	O	S	0	0	0
			2424	1562	408	439	15			
1	I	288	Total	C	N	O	S	0	0	0
			2443	1575	411	442	15			
1	K	288	Total	C	N	O	S	0	0	0
			2443	1575	411	442	15			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	203	TYR	CYS	engineered mutation	UNP Q8IFM5
A	216	ALA	THR	engineered mutation	UNP Q8IFM5
A	299	ALA	THR	engineered mutation	UNP Q8IFM5
C	203	TYR	CYS	engineered mutation	UNP Q8IFM5
C	216	ALA	THR	engineered mutation	UNP Q8IFM5
C	299	ALA	THR	engineered mutation	UNP Q8IFM5
E	203	TYR	CYS	engineered mutation	UNP Q8IFM5
E	216	ALA	THR	engineered mutation	UNP Q8IFM5
E	299	ALA	THR	engineered mutation	UNP Q8IFM5
G	203	TYR	CYS	engineered mutation	UNP Q8IFM5
G	216	ALA	THR	engineered mutation	UNP Q8IFM5
G	299	ALA	THR	engineered mutation	UNP Q8IFM5
I	203	TYR	CYS	engineered mutation	UNP Q8IFM5
I	216	ALA	THR	engineered mutation	UNP Q8IFM5
I	299	ALA	THR	engineered mutation	UNP Q8IFM5
K	203	TYR	CYS	engineered mutation	UNP Q8IFM5
K	216	ALA	THR	engineered mutation	UNP Q8IFM5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
K	299	ALA	THR	engineered mutation	UNP Q8IFM5

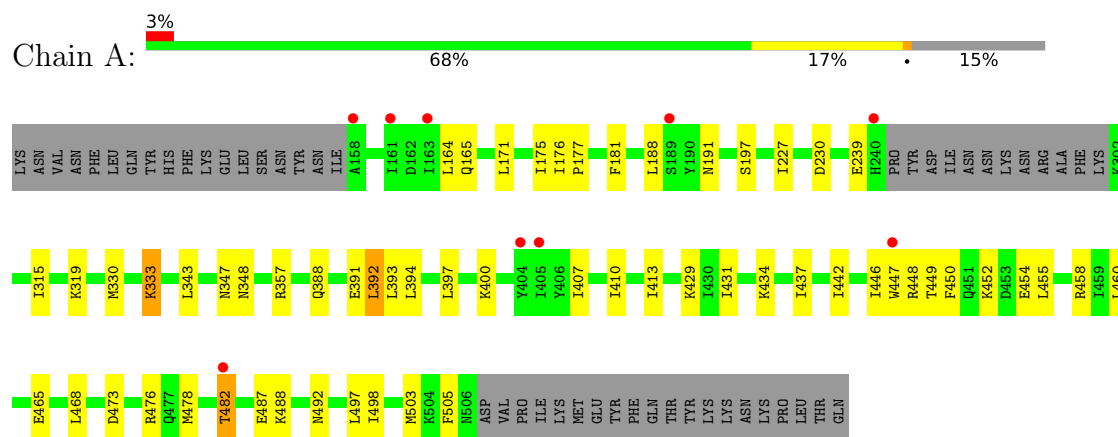
- Molecule 2 is a protein called monoclonal antibody MAD10-255.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	223	Total	C	N	O	S	0	1	0
			1736	1099	288	343	6			
2	D	226	Total	C	N	O	S	0	1	0
			1756	1109	291	350	6			
2	F	226	Total	C	N	O	S	0	1	0
			1756	1109	291	350	6			
2	H	226	Total	C	N	O	S	0	1	0
			1756	1109	291	350	6			
2	J	222	Total	C	N	O	S	0	1	0
			1728	1093	287	342	6			

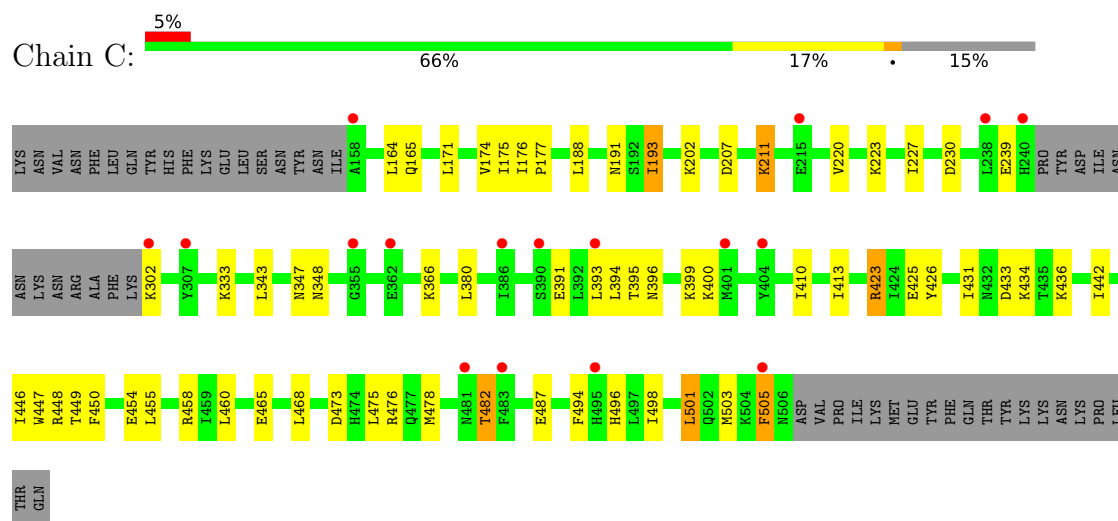
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

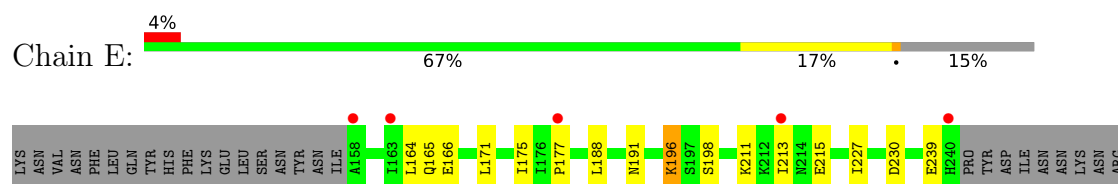
• Molecule 1: Reticulocyte-binding protein homolog 5

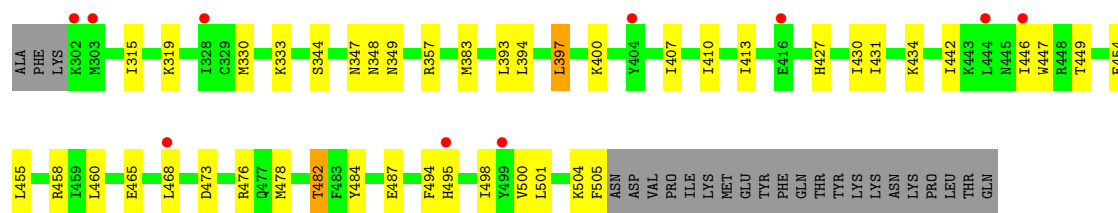


• Molecule 1: Reticulocyte-binding protein homolog 5

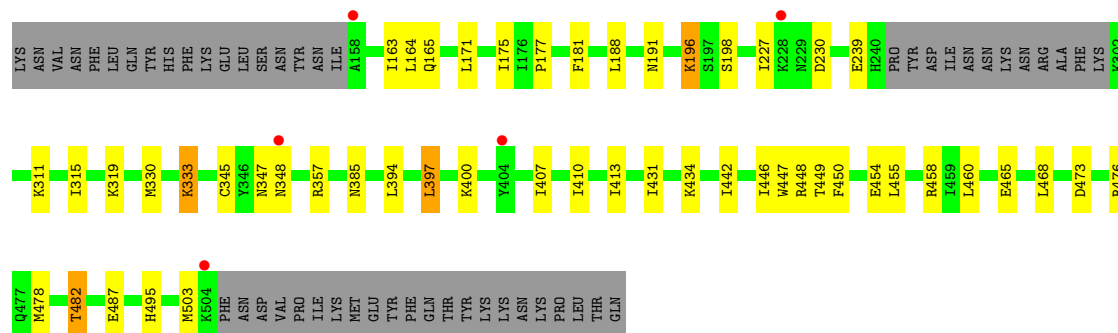


• Molecule 1: Reticulocyte-binding protein homolog 5

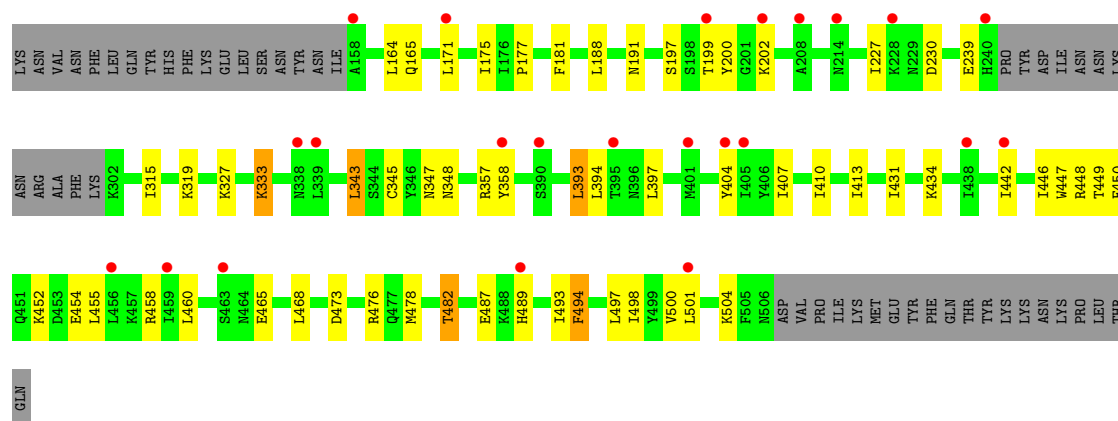




• Molecule 1: Reticulocyte-binding protein homolog 5

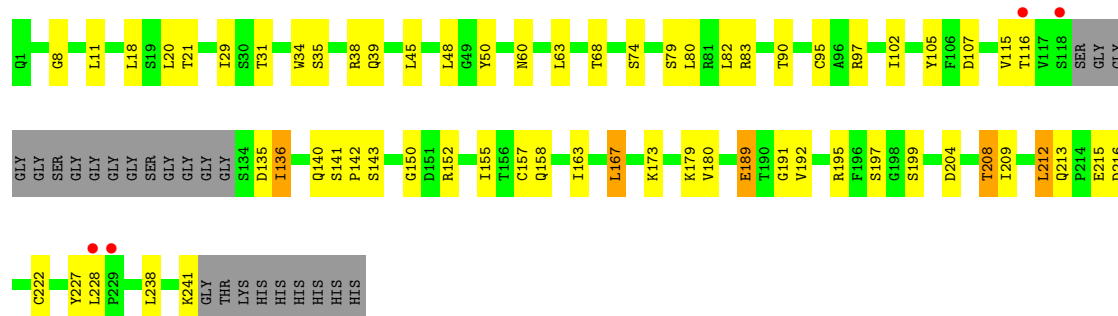
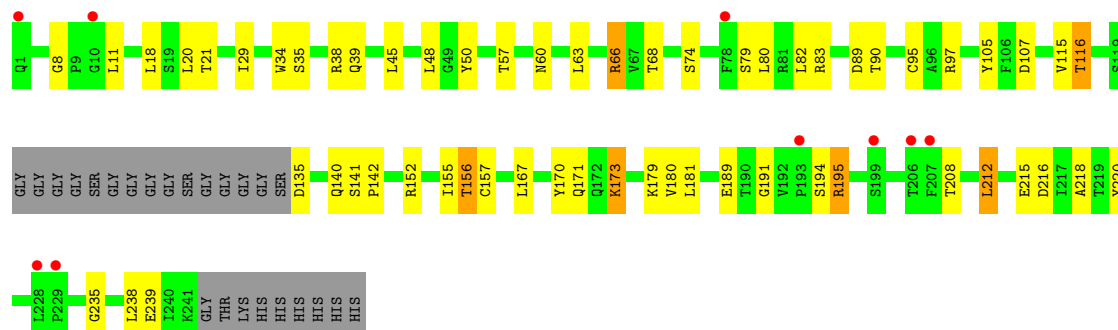
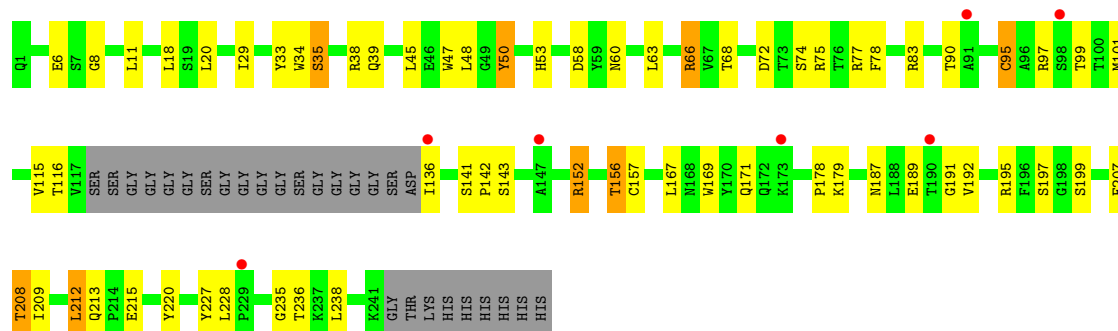


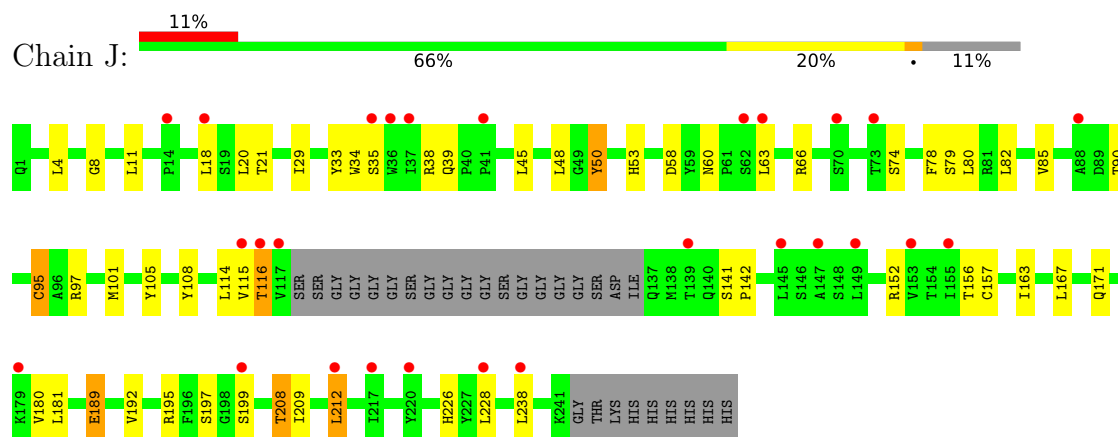
• Molecule 1: Reticulocyte-binding protein homolog 5



• Molecule 1: Reticulocyte-binding protein homolog 5







4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	115.31Å 134.52Å 198.67Å 90.00° 93.56° 90.00°	Depositor
Resolution (Å)	87.45 – 3.15 87.45 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.8 (87.45-3.15) 99.8 (87.45-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 3.13Å)	Xtriage
Refinement program	BUSTER 2.10.4 (20-OCT-2021)	Depositor
R, R_{free}	0.242 , 0.264 0.245 , 0.265	Depositor DCC
R_{free} test set	5485 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	102.5	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 108.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	23363	wwPDB-VP
Average B, all atoms (Å ²)	136.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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 [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	0.44	0/2493	0.59	0/3342
1	C	0.44	0/2493	0.60	0/3342
1	E	0.44	0/2485	0.61	0/3331
1	G	0.44	0/2473	0.59	0/3315
1	I	0.33	0/2493	0.56	0/3342
1	K	0.32	0/2493	0.54	0/3342
2	B	0.51	0/1781	0.72	0/2426
2	D	0.51	0/1801	0.72	0/2453
2	F	0.49	0/1801	0.71	0/2453
2	H	0.49	0/1801	0.71	0/2453
2	J	0.34	0/1773	0.62	0/2415
All	All	0.43	0/23887	0.63	0/32214

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2443	0	2465	44	0
1	C	2443	0	2465	41	0
1	E	2435	0	2459	41	0
1	G	2424	0	2450	41	0
1	I	2443	0	2465	36	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	2443	0	2465	30	0
2	B	1736	0	1690	35	0
2	D	1756	0	1704	29	0
2	F	1756	0	1704	32	0
2	H	1756	0	1704	31	0
2	J	1728	0	1679	32	0
All	All	23363	0	23250	353	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 8.

All (353) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:163:ILE:HG23	1:G:171:LEU:HD21	1.22	1.10
2:D:29:ILE:HG23	2:D:34:TRP:NE1	1.83	0.93
1:E:196:LYS:NZ	1:E:198:SER:HB3	1.83	0.93
2:F:29:ILE:HG23	2:F:34:TRP:NE1	1.83	0.92
2:H:29:ILE:HG23	2:H:34:TRP:NE1	1.86	0.91
1:E:196:LYS:HZ2	1:E:198:SER:HB3	1.36	0.91
1:I:446:ILE:HG23	1:I:447:TRP:CD1	2.06	0.91
1:C:503:MET:HA	1:E:400:LYS:NZ	1.86	0.91
1:K:446:ILE:HG23	1:K:447:TRP:CD1	2.06	0.90
1:G:446:ILE:HG23	1:G:447:TRP:CD1	2.07	0.90
1:C:446:ILE:HG23	1:C:447:TRP:CD1	2.07	0.90
1:E:446:ILE:HG23	1:E:447:TRP:CD1	2.07	0.89
1:A:503:MET:HA	1:G:400:LYS:NZ	1.88	0.89
1:A:446:ILE:HG23	1:A:447:TRP:CD1	2.07	0.88
1:G:196:LYS:NZ	1:G:198:SER:HB3	1.88	0.88
1:G:196:LYS:HZ2	1:G:198:SER:HB3	1.41	0.84
1:A:392:LEU:HG	1:I:358:TYR:CD2	2.13	0.83
1:C:207:ASP:O	1:C:211:LYS:HD2	1.79	0.83
1:C:393:LEU:HD12	1:E:495:HIS:CD2	2.14	0.82
2:B:8:GLY:HA3	2:B:20:LEU:HD23	1.62	0.82
2:B:29:ILE:HG23	2:B:34:TRP:NE1	1.95	0.82
1:A:400:LYS:NZ	1:G:503:MET:HG2	1.94	0.82
2:B:75:ARG:HG2	2:B:77:ARG:HD2	1.63	0.80
1:A:392:LEU:HG	1:I:358:TYR:CE2	2.18	0.79
1:A:400:LYS:HZ3	1:G:503:MET:HG2	1.45	0.78
2:B:191:GLY:HA3	1:C:347:ASN:HB2	1.66	0.77
1:A:503:MET:HA	1:G:400:LYS:HZ3	1.50	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:503:MET:HA	1:E:400:LYS:HZ3	1.48	0.76
1:A:393:LEU:HD12	1:G:495:HIS:HD2	1.54	0.72
1:G:163:ILE:CG2	1:G:171:LEU:HD21	2.13	0.72
1:K:500:VAL:HA	1:K:503:MET:HG3	1.74	0.69
1:E:165:GLN:HG3	1:E:171:LEU:HD23	1.75	0.69
1:I:500:VAL:O	1:I:504:LYS:HG2	1.94	0.68
2:H:8:GLY:HA3	2:H:20:LEU:HD23	1.77	0.67
2:B:212:LEU:HD21	2:B:238:LEU:HD21	1.76	0.67
2:D:212:LEU:HD21	2:D:238:LEU:HD21	1.78	0.66
2:D:171:GLN:HB2	2:D:181:LEU:HD11	1.78	0.66
2:H:212:LEU:HD21	2:H:238:LEU:HD21	1.77	0.65
2:F:8:GLY:HA3	2:F:20:LEU:HD23	1.77	0.65
2:D:60:ASN:HB3	2:D:63:LEU:HD23	1.78	0.65
2:F:191:GLY:HA3	1:G:347:ASN:HB2	1.79	0.65
1:C:498:ILE:HG12	1:E:498:ILE:HG12	1.80	0.64
2:F:212:LEU:HD21	2:F:238:LEU:HD21	1.78	0.64
2:J:212:LEU:HD21	2:J:238:LEU:HD21	1.79	0.64
2:D:90:THR:HG23	2:D:116:THR:HG22	1.78	0.64
1:G:239:GLU:HG2	1:G:413:ILE:HD11	1.80	0.64
1:C:501:LEU:HB3	1:E:501:LEU:HD23	1.80	0.63
2:D:8:GLY:HA3	2:D:20:LEU:HD23	1.80	0.63
1:I:165:GLN:HG3	1:I:171:LEU:HD23	1.81	0.63
2:J:29:ILE:HG23	2:J:34:TRP:NE1	2.14	0.62
1:A:347:ASN:HB2	2:D:191:GLY:HA3	1.81	0.62
2:J:90:THR:HG23	2:J:116:THR:HG22	1.82	0.62
1:A:165:GLN:HG3	1:A:171:LEU:HD23	1.81	0.62
1:A:393:LEU:HD12	1:G:495:HIS:CD2	2.33	0.62
1:A:388:GLN:HG2	1:I:197:SER:HB2	1.82	0.62
1:C:175:ILE:HG22	1:C:177:PRO:HD2	1.81	0.62
1:C:393:LEU:HD12	1:E:495:HIS:HD2	1.64	0.62
2:J:8:GLY:HA3	2:J:20:LEU:HD23	1.81	0.62
1:E:347:ASN:HB2	2:H:191:GLY:HA3	1.81	0.62
1:K:165:GLN:HG3	1:K:171:LEU:HD23	1.81	0.62
2:B:189:GLU:O	2:B:192:VAL:HG12	2.00	0.61
1:C:220:VAL:HA	1:C:223:LYS:HE3	1.83	0.61
1:E:196:LYS:HZ3	1:E:198:SER:HB3	1.65	0.61
1:E:239:GLU:HG2	1:E:413:ILE:HD11	1.84	0.60
1:A:239:GLU:HG2	1:A:413:ILE:HD11	1.83	0.60
1:I:239:GLU:HG2	1:I:413:ILE:HD11	1.83	0.60
1:K:239:GLU:HG2	1:K:413:ILE:HD11	1.84	0.60
1:A:454:GLU:O	1:A:458:ARG:HG2	2.02	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:165:GLN:HG3	1:G:171:LEU:HD23	1.83	0.59
2:H:197:SER:HB2	2:H:208:THR:HG23	1.84	0.59
2:F:141:SER:HB2	2:F:142:PRO:HD3	1.84	0.58
2:J:141:SER:HB2	2:J:142:PRO:HD3	1.85	0.58
1:A:503:MET:HA	1:G:400:LYS:HZ2	1.67	0.58
1:C:239:GLU:HG2	1:C:413:ILE:HD11	1.85	0.58
2:H:217:ILE:HG23	2:H:239:GLU:HA	1.85	0.58
2:J:197:SER:HB2	2:J:208:THR:HG23	1.86	0.58
1:E:213:ILE:HD13	2:F:102:ILE:HG13	1.86	0.57
2:B:197:SER:HB2	2:B:208:THR:HG23	1.85	0.57
1:G:196:LYS:HZ3	1:G:198:SER:HB3	1.68	0.57
2:B:72:ASP:OD2	2:B:75:ARG:HB2	2.03	0.57
2:B:58:ASP:HB3	2:B:228:LEU:HD11	1.87	0.56
2:H:189:GLU:O	2:H:192:VAL:HG12	2.05	0.56
2:F:197:SER:HB2	2:F:208:THR:HG23	1.87	0.56
1:G:397:LEU:HD23	1:G:407:ILE:HG22	1.87	0.56
1:A:397:LEU:HD23	1:A:407:ILE:HG22	1.87	0.56
2:J:97:ARG:NH1	2:J:108:TYR:HE2	2.04	0.55
1:E:427:HIS:HA	1:E:430:ILE:HD12	1.88	0.55
2:J:163:ILE:HG23	2:J:226:HIS:HB2	1.87	0.55
2:B:29:ILE:HG23	2:B:34:TRP:CD1	2.42	0.55
2:F:158:GLN:NE2	2:F:204:ASP:OD1	2.32	0.54
2:B:60:ASN:HB3	2:B:63:LEU:HD23	1.90	0.54
2:H:66:ARG:NH2	2:H:89:ASP:OD2	2.42	0.53
1:I:315:ILE:HG22	1:I:319:LYS:HE2	1.90	0.53
1:A:315:ILE:HG22	1:A:319:LYS:HE2	1.89	0.53
2:F:60:ASN:HB3	2:F:63:LEU:HD23	1.90	0.53
1:I:393:LEU:HD22	1:I:494:PHE:CE1	2.44	0.53
1:E:330:MET:CE	2:F:31:THR:HG21	2.39	0.53
1:C:395:THR:HG21	1:K:200:TYR:HB3	1.91	0.53
1:E:397:LEU:HD23	1:E:407:ILE:HG22	1.90	0.53
2:F:105:TYR:HD1	2:F:180:VAL:HG21	1.74	0.53
2:F:189:GLU:O	2:F:192:VAL:HG12	2.09	0.53
1:A:448:ARG:NH1	1:A:450:PHE:CD1	2.77	0.52
1:E:211:LYS:O	1:E:215:GLU:HG3	2.09	0.52
2:H:60:ASN:HB3	2:H:63:LEU:HD23	1.90	0.52
2:D:90:THR:CG2	2:D:116:THR:HG22	2.39	0.52
1:E:383:MET:HE3	1:E:484:TYR:HE2	1.74	0.52
1:K:315:ILE:HG22	1:K:319:LYS:HE2	1.91	0.52
1:I:397:LEU:HD23	1:I:407:ILE:HG22	1.92	0.52
2:J:189:GLU:O	2:J:192:VAL:HG12	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:LEU:HD22	1:A:478:MET:HB3	1.93	0.51
1:C:505:PHE:HZ	1:E:504:LYS:HB2	1.73	0.51
2:D:29:ILE:HG23	2:D:34:TRP:CD1	2.46	0.51
1:E:315:ILE:HG22	1:E:319:LYS:HE2	1.92	0.51
1:E:164:LEU:HD22	1:E:478:MET:HB3	1.93	0.51
2:F:20:LEU:HD12	2:F:80:LEU:HD23	1.93	0.51
2:B:169:TRP:CE2	2:B:207:PHE:HB2	2.46	0.51
2:B:35:SER:HB3	2:B:50:TYR:HB3	1.92	0.51
1:K:397:LEU:HD23	1:K:407:ILE:HG22	1.93	0.51
1:K:491:ASN:HA	1:K:494:PHE:HB2	1.93	0.51
1:I:199:THR:HG23	1:I:202:LYS:HB3	1.92	0.51
1:G:315:ILE:HG22	1:G:319:LYS:HE2	1.91	0.51
1:C:380:LEU:HD13	1:C:425:GLU:HG3	1.93	0.50
1:E:394:LEU:HD23	1:E:410:ILE:HG22	1.93	0.50
1:K:164:LEU:HD22	1:K:478:MET:HB3	1.93	0.50
2:H:163:ILE:HD13	2:H:226:HIS:HB3	1.93	0.50
1:I:404:TYR:HE1	1:I:504:LYS:HE3	1.76	0.50
1:A:400:LYS:HZ3	1:G:503:MET:CG	2.22	0.50
1:G:164:LEU:HD22	1:G:478:MET:HB3	1.92	0.50
1:K:394:LEU:HD23	1:K:410:ILE:HG22	1.93	0.50
2:B:152:ARG:NH1	2:F:150:GLY:O	2.43	0.50
1:C:498:ILE:HG21	1:E:393:LEU:HD11	1.92	0.50
2:D:39:GLN:HB2	2:D:45:LEU:HD23	1.93	0.50
1:C:176:ILE:HD12	1:C:475:LEU:HD13	1.94	0.50
1:I:394:LEU:HD23	1:I:410:ILE:HG22	1.93	0.50
2:J:97:ARG:NH1	2:J:108:TYR:CE2	2.79	0.50
2:B:63:LEU:O	2:B:66:ARG:HG2	2.11	0.49
1:A:347:ASN:O	1:A:348:ASN:HB2	2.11	0.49
1:G:448:ARG:NH1	1:G:450:PHE:CD1	2.80	0.49
2:H:142:PRO:HD2	2:H:155:ILE:HG23	1.94	0.49
1:I:494:PHE:O	1:I:498:ILE:HG13	2.12	0.49
2:J:90:THR:CG2	2:J:116:THR:HG22	2.42	0.49
1:I:164:LEU:HD22	1:I:478:MET:HB3	1.93	0.49
1:E:347:ASN:O	1:E:348:ASN:HB2	2.12	0.49
1:I:227:ILE:HD12	1:I:227:ILE:H	1.77	0.49
2:J:20:LEU:HD12	2:J:80:LEU:HD23	1.94	0.49
1:E:227:ILE:HD12	1:E:227:ILE:H	1.77	0.49
2:D:141:SER:HB2	2:D:156:THR:OG1	2.11	0.49
1:I:448:ARG:NH1	1:I:450:PHE:CD1	2.81	0.49
2:B:39:GLN:HB2	2:B:45:LEU:HD23	1.95	0.49
2:H:20:LEU:HD12	2:H:80:LEU:HD23	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:29:ILE:HG23	2:H:34:TRP:CD1	2.46	0.49
2:J:60:ASN:HB3	2:J:63:LEU:HD23	1.94	0.49
1:C:227:ILE:HD12	1:C:227:ILE:H	1.78	0.49
1:C:494:PHE:O	1:C:498:ILE:HG13	2.13	0.49
1:C:448:ARG:NH1	1:C:450:PHE:CD1	2.81	0.48
1:G:227:ILE:HD12	1:G:227:ILE:H	1.78	0.48
1:G:347:ASN:O	1:G:348:ASN:HB2	2.13	0.48
1:K:494:PHE:O	1:K:498:ILE:HG13	2.13	0.48
1:C:394:LEU:HD23	1:C:410:ILE:HG22	1.95	0.48
2:F:29:ILE:HG23	2:F:34:TRP:CD1	2.47	0.48
2:F:142:PRO:HD2	2:F:155:ILE:HG23	1.94	0.48
1:A:388:GLN:HG2	1:I:197:SER:CB	2.42	0.48
1:C:347:ASN:O	1:C:348:ASN:HB2	2.14	0.48
1:K:448:ARG:NH1	1:K:450:PHE:CD1	2.81	0.48
1:I:410:ILE:HD11	1:I:493:ILE:HB	1.95	0.48
1:A:227:ILE:H	1:A:227:ILE:HD12	1.79	0.48
2:F:39:GLN:HB2	2:F:45:LEU:HD23	1.95	0.48
1:G:188:LEU:HD11	1:G:460:LEU:HD23	1.96	0.48
1:K:195:HIS:CD2	1:K:343:LEU:CD1	2.97	0.48
1:A:394:LEU:HD23	1:A:410:ILE:HG22	1.96	0.48
2:B:136:ILE:HD13	2:B:227:TYR:HB2	1.95	0.48
1:C:448:ARG:HH11	1:C:448:ARG:HB3	1.79	0.48
1:G:163:ILE:HD13	1:G:311:LYS:HE3	1.96	0.48
2:H:39:GLN:HB2	2:H:45:LEU:HD23	1.95	0.48
2:J:78:PHE:CZ	2:J:95:CYS:SG	3.06	0.48
2:D:66:ARG:NH2	2:D:89:ASP:OD2	2.47	0.48
1:G:434:LYS:HE2	1:G:468:LEU:HD12	1.96	0.48
1:I:347:ASN:O	1:I:348:ASN:HB2	2.14	0.48
2:J:39:GLN:HB2	2:J:45:LEU:HD23	1.96	0.48
1:A:400:LYS:NZ	1:G:503:MET:CG	2.71	0.47
2:D:105:TYR:HD1	2:D:180:VAL:HG21	1.78	0.47
1:G:442:ILE:HG13	1:G:446:ILE:HD12	1.96	0.47
1:K:227:ILE:H	1:K:227:ILE:HD12	1.78	0.47
2:B:78:PHE:CZ	2:B:95:CYS:SG	3.08	0.47
2:D:20:LEU:HD12	2:D:80:LEU:HD23	1.95	0.47
2:B:33:TYR:CE2	2:B:101:MET:HG2	2.49	0.47
2:D:63:LEU:O	2:D:66:ARG:HG2	2.14	0.47
1:A:488:LYS:HE2	1:A:492:ASN:HD21	1.80	0.47
1:C:442:ILE:HG13	1:C:446:ILE:HD12	1.96	0.47
1:E:442:ILE:HG13	1:E:446:ILE:HD12	1.97	0.47
1:A:442:ILE:HG13	1:A:446:ILE:HD12	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:448:ARG:HD3	1:C:450:PHE:CZ	2.50	0.47
2:D:195:ARG:NH1	2:D:216:ASP:OD1	2.43	0.47
2:J:34:TRP:CZ3	2:J:97:ARG:HB2	2.50	0.47
2:J:82:LEU:HD12	2:J:85:VAL:HG12	1.97	0.47
2:H:195:ARG:HG3	2:H:209:ILE:HG23	1.97	0.47
1:I:343:LEU:O	1:I:452:LYS:HE3	2.14	0.47
1:A:188:LEU:HD11	1:A:460:LEU:HD23	1.95	0.47
1:C:431:ILE:HD11	1:C:473:ASP:HA	1.97	0.47
1:I:442:ILE:HG13	1:I:446:ILE:HD12	1.96	0.47
2:J:29:ILE:HG23	2:J:34:TRP:CD1	2.50	0.47
1:C:188:LEU:HD11	1:C:460:LEU:HD23	1.97	0.46
1:E:431:ILE:HD11	1:E:473:ASP:HA	1.97	0.46
1:A:448:ARG:HD3	1:A:450:PHE:CZ	2.50	0.46
1:C:165:GLN:HG3	1:C:171:LEU:HD23	1.96	0.46
1:C:434:LYS:HE2	1:C:468:LEU:HD12	1.98	0.46
1:E:494:PHE:O	1:E:498:ILE:HG13	2.15	0.46
2:J:4:LEU:HD21	2:J:34:TRP:HZ3	1.80	0.46
1:K:343:LEU:O	1:K:452:LYS:HE3	2.16	0.46
2:D:18:LEU:HD13	2:D:115:VAL:HG11	1.97	0.46
1:G:394:LEU:HD23	1:G:410:ILE:HG22	1.97	0.46
1:G:454:GLU:O	1:G:458:ARG:HG2	2.16	0.46
2:D:141:SER:HB2	2:D:142:PRO:HD3	1.97	0.46
1:I:404:TYR:CE1	1:I:504:LYS:HE3	2.50	0.46
1:E:434:LYS:HE2	1:E:468:LEU:HD12	1.98	0.45
2:F:90:THR:HG23	2:F:116:THR:HA	1.99	0.45
1:G:448:ARG:HD3	1:G:450:PHE:CZ	2.51	0.45
1:K:442:ILE:HG13	1:K:446:ILE:HD12	1.97	0.45
1:E:383:MET:HE3	1:E:484:TYR:CE2	2.51	0.45
1:G:175:ILE:HG22	1:G:177:PRO:HD2	1.98	0.45
2:B:171:GLN:HG3	2:B:220:TYR:CE2	2.51	0.45
1:C:399:LYS:HG3	1:C:400:LYS:HG3	1.98	0.45
1:E:330:MET:HE2	2:F:31:THR:HG21	1.99	0.45
1:G:448:ARG:HH11	1:G:448:ARG:HB3	1.81	0.45
2:H:63:LEU:HD12	2:H:82:LEU:HD11	1.98	0.45
1:I:454:GLU:O	1:I:458:ARG:HG2	2.17	0.45
1:K:188:LEU:HD11	1:K:460:LEU:HD23	1.98	0.45
1:K:454:GLU:O	1:K:458:ARG:HG2	2.16	0.45
1:I:175:ILE:HG22	1:I:177:PRO:HD2	1.97	0.45
1:I:448:ARG:HH11	1:I:448:ARG:HB3	1.82	0.45
1:A:400:LYS:HZ1	1:G:503:MET:HG2	1.81	0.45
2:H:66:ARG:HH22	2:H:89:ASP:CG	2.19	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:188:LEU:HD11	1:I:460:LEU:HD23	1.98	0.45
2:J:18:LEU:HD13	2:J:115:VAL:HG11	1.99	0.45
1:A:175:ILE:HG22	1:A:177:PRO:HD2	1.99	0.45
2:B:18:LEU:HD13	2:B:115:VAL:HG11	1.97	0.45
2:B:195:ARG:HG3	2:B:209:ILE:HG23	1.99	0.45
1:C:478:MET:O	1:C:482:THR:HG23	2.17	0.45
2:D:195:ARG:NH1	2:D:216:ASP:OD2	2.50	0.45
1:E:175:ILE:HG22	1:E:177:PRO:HD2	1.99	0.45
1:A:431:ILE:HD11	1:A:473:ASP:HA	1.99	0.45
2:J:195:ARG:HG3	2:J:209:ILE:HG23	1.99	0.45
2:B:6:GLU:OE1	2:B:95:CYS:HB3	2.17	0.44
2:H:141:SER:HB2	2:H:142:PRO:HD3	1.98	0.44
1:A:478:MET:O	1:A:482:THR:HG23	2.17	0.44
2:B:68:THR:OG1	2:B:83:ARG:NH2	2.50	0.44
1:E:454:GLU:O	1:E:458:ARG:HG2	2.17	0.44
2:F:38:ARG:HG2	2:F:48:LEU:HD21	1.99	0.44
1:I:489:HIS:O	1:I:493:ILE:HG13	2.17	0.44
1:K:175:ILE:HG22	1:K:177:PRO:HD2	1.99	0.44
1:E:500:VAL:O	1:E:504:LYS:HG2	2.18	0.44
2:H:38:ARG:HG2	2:H:48:LEU:HD21	1.98	0.44
1:I:431:ILE:HD11	1:I:473:ASP:HA	1.98	0.44
1:E:188:LEU:HD11	1:E:460:LEU:HD23	1.99	0.44
1:G:163:ILE:HG23	1:G:171:LEU:CD2	2.16	0.44
1:K:202:LYS:HG3	1:K:202:LYS:O	2.18	0.44
1:C:433:ASP:HA	1:C:436:LYS:HD2	1.99	0.44
2:F:18:LEU:HD13	2:F:115:VAL:HG11	2.00	0.44
2:J:114:LEU:HD11	2:J:116:THR:HG23	1.98	0.44
1:K:448:ARG:HD3	1:K:450:PHE:CZ	2.52	0.44
1:E:478:MET:O	1:E:482:THR:HG23	2.18	0.44
2:F:63:LEU:HD12	2:F:82:LEU:HD11	2.00	0.44
1:A:393:LEU:CD1	1:G:495:HIS:CD2	2.99	0.44
2:D:68:THR:OG1	2:D:83:ARG:NH2	2.50	0.44
2:F:29:ILE:HG23	2:F:34:TRP:HE1	1.74	0.44
2:F:195:ARG:NH1	2:F:216:ASP:OD2	2.47	0.44
2:J:33:TYR:CE2	2:J:101:MET:HG2	2.52	0.44
1:K:431:ILE:HD11	1:K:473:ASP:HA	1.98	0.44
2:B:142:PRO:O	2:B:236:THR:HG23	2.18	0.44
2:B:90:THR:HG23	2:B:116:THR:HA	1.99	0.44
2:H:220:TYR:O	2:H:235:GLY:HA2	2.18	0.44
1:K:448:ARG:HH11	1:K:448:ARG:HB3	1.82	0.44
1:A:448:ARG:HB3	1:A:448:ARG:HH11	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:LYS:HE2	1:A:468:LEU:HD12	1.99	0.43
2:D:29:ILE:HG23	2:D:34:TRP:HE1	1.74	0.43
2:J:105:TYR:HD1	2:J:180:VAL:HG21	1.83	0.43
1:G:330:MET:CE	2:H:31:THR:HG21	2.48	0.43
2:J:38:ARG:HG2	2:J:48:LEU:HD21	2.00	0.43
1:I:448:ARG:HD3	1:I:450:PHE:CZ	2.53	0.43
1:K:195:HIS:CD2	1:K:343:LEU:HD11	2.53	0.43
2:B:35:SER:HB3	2:B:47:TRP:HE1	1.83	0.43
1:E:330:MET:HE3	2:F:31:THR:HG21	2.00	0.43
1:G:431:ILE:HD11	1:G:473:ASP:HA	1.98	0.43
1:I:327:LYS:HG2	2:J:53:HIS:HE1	1.83	0.43
2:F:195:ARG:HG3	2:F:209:ILE:HG23	2.01	0.43
2:H:18:LEU:HD13	2:H:115:VAL:HG11	2.00	0.43
2:D:63:LEU:HD12	2:D:82:LEU:HD11	2.00	0.43
2:H:29:ILE:HG23	2:H:34:TRP:HE1	1.76	0.43
1:I:478:MET:O	1:I:482:THR:HG23	2.18	0.43
2:D:38:ARG:HG2	2:D:48:LEU:HD21	2.00	0.43
2:H:78:PHE:CZ	2:H:95:CYS:SG	3.11	0.43
2:J:50:TYR:CE1	2:J:58:ASP:HB2	2.54	0.43
1:K:478:MET:O	1:K:482:THR:HG23	2.18	0.43
1:C:164:LEU:HD22	1:C:478:MET:HB3	1.99	0.43
2:D:170:TYR:CE2	2:D:180:VAL:HG22	2.54	0.43
1:G:478:MET:O	1:G:482:THR:HG23	2.19	0.43
1:K:181:PHE:CZ	1:K:333:LYS:HB2	2.54	0.43
1:A:343:LEU:O	1:A:452:LYS:HE3	2.18	0.42
2:B:141:SER:HB2	2:B:156:THR:OG1	2.19	0.42
1:I:434:LYS:HE2	1:I:468:LEU:HD12	2.01	0.42
1:K:393:LEU:HD22	1:K:494:PHE:CE1	2.54	0.42
2:D:90:THR:HG23	2:D:116:THR:HA	2.01	0.42
2:B:29:ILE:HA	2:B:34:TRP:CZ2	2.55	0.42
1:C:396:ASN:HA	1:C:399:LYS:HG2	2.02	0.42
2:H:90:THR:HG23	2:H:116:THR:HA	2.01	0.42
2:B:38:ARG:HG2	2:B:48:LEU:HD21	2.01	0.42
2:F:142:PRO:HG2	2:F:155:ILE:HA	2.01	0.42
2:H:98:SER:HB3	2:H:104:GLN:HE21	1.84	0.42
1:K:496:HIS:ND1	1:K:497:LEU:HD23	2.34	0.42
1:E:347:ASN:HD22	1:E:349:ASN:HB2	1.84	0.42
2:D:142:PRO:HD2	2:D:155:ILE:HG23	2.02	0.42
2:F:29:ILE:HG23	2:F:34:TRP:CE2	2.52	0.42
1:G:181:PHE:CZ	1:G:333:LYS:HB2	2.55	0.42
2:J:97:ARG:HD2	2:J:108:TYR:HD2	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:212:LEU:HD22	2:B:212:LEU:HA	1.96	0.41
1:I:181:PHE:CZ	1:I:333:LYS:HB2	2.54	0.41
2:J:171:GLN:HB2	2:J:181:LEU:HD11	2.01	0.41
1:C:174:VAL:HG11	1:C:475:LEU:HD21	2.03	0.41
1:E:166:GLU:HG2	1:E:482:THR:HG22	2.01	0.41
1:C:393:LEU:CD1	1:E:495:HIS:CD2	2.96	0.41
2:F:136:ILE:HD13	2:F:227:TYR:HB2	2.01	0.41
2:H:63:LEU:O	2:H:66:ARG:HG2	2.20	0.41
2:H:136:ILE:HD13	2:H:227:TYR:HB2	2.01	0.41
1:A:181:PHE:CZ	1:A:333:LYS:HB2	2.56	0.41
2:B:220:TYR:O	2:B:235:GLY:HA2	2.20	0.41
1:C:193:ILE:HG22	1:C:202:LYS:HD3	2.01	0.41
1:A:330:MET:HB3	2:B:53:HIS:CE1	2.56	0.41
1:A:434:LYS:HD3	1:A:437:ILE:HD12	2.02	0.41
2:H:68:THR:OG1	2:H:83:ARG:NH2	2.54	0.41
2:B:178:PRO:O	2:B:179:LYS:HD3	2.21	0.41
1:C:176:ILE:HD12	1:C:475:LEU:CD1	2.50	0.41
1:A:434:LYS:HD3	1:A:434:LYS:HA	1.92	0.41
2:B:191:GLY:HA3	1:C:347:ASN:CB	2.46	0.41
2:D:220:TYR:O	2:D:235:GLY:HA2	2.21	0.41
2:H:141:SER:HB2	2:H:156:THR:OG1	2.21	0.41
2:J:63:LEU:HD12	2:J:82:LEU:HD21	2.03	0.41
2:J:90:THR:HG23	2:J:116:THR:HA	2.03	0.41
1:A:176:ILE:HB	1:A:177:PRO:HD3	2.03	0.40
1:C:423:ARG:NH1	1:C:426:TYR:CD2	2.89	0.40
2:D:173:LYS:HE2	2:D:218:ALA:HB2	2.03	0.40
2:F:29:ILE:HA	2:F:34:TRP:CZ2	2.56	0.40
2:F:167:LEU:HD11	2:F:222:CYS:HB2	2.02	0.40
2:J:90:THR:HG23	2:J:116:THR:CG2	2.51	0.40
1:K:434:LYS:HE2	1:K:468:LEU:HD12	2.02	0.40
1:C:454:GLU:O	1:C:458:ARG:HG2	2.22	0.40
1:A:503:MET:SD	1:G:400:LYS:NZ	2.88	0.40
2:D:29:ILE:HA	2:D:34:TRP:CZ2	2.55	0.40
1:A:429:LYS:HE2	1:A:429:LYS:HB3	1.88	0.40
2:F:68:THR:OG1	2:F:83:ARG:NH2	2.54	0.40
2:H:105:TYR:CD1	2:H:180:VAL:HG21	2.56	0.40
1:I:404:TYR:OH	1:I:501:LEU:HA	2.22	0.40
1:I:410:ILE:HG21	1:I:494:PHE:HE1	1.85	0.40
1:K:429:LYS:HE2	1:K:429:LYS:HB3	1.86	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	284/338 (84%)	269 (95%)	15 (5%)	0	100	100
1	C	284/338 (84%)	268 (94%)	16 (6%)	0	100	100
1	E	283/338 (84%)	271 (96%)	12 (4%)	0	100	100
1	G	282/338 (83%)	265 (94%)	17 (6%)	0	100	100
1	I	284/338 (84%)	264 (93%)	20 (7%)	0	100	100
1	K	284/338 (84%)	267 (94%)	17 (6%)	0	100	100
2	B	220/250 (88%)	201 (91%)	19 (9%)	0	100	100
2	D	223/250 (89%)	206 (92%)	17 (8%)	0	100	100
2	F	223/250 (89%)	202 (91%)	21 (9%)	0	100	100
2	H	223/250 (89%)	203 (91%)	20 (9%)	0	100	100
2	J	219/250 (88%)	202 (92%)	17 (8%)	0	100	100
All	All	2809/3278 (86%)	2618 (93%)	191 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	278/327 (85%)	262 (94%)	16 (6%)	17	41
1	C	278/327 (85%)	259 (93%)	19 (7%)	13	36
1	E	277/327 (85%)	263 (95%)	14 (5%)	20	45

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	276/327 (84%)	262 (95%)	14 (5%)	20	45
1	I	278/327 (85%)	262 (94%)	16 (6%)	17	41
1	K	278/327 (85%)	262 (94%)	16 (6%)	17	41
2	B	195/208 (94%)	176 (90%)	19 (10%)	6	23
2	D	198/208 (95%)	171 (86%)	27 (14%)	3	12
2	F	198/208 (95%)	171 (86%)	27 (14%)	3	12
2	H	198/208 (95%)	173 (87%)	25 (13%)	3	14
2	J	194/208 (93%)	176 (91%)	18 (9%)	7	25
All	All	2648/3002 (88%)	2437 (92%)	211 (8%)	10	31

All (211) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	191	ASN
1	A	197	SER
1	A	230	ASP
1	A	333	LYS
1	A	357	ARG
1	A	391	GLU
1	A	392	LEU
1	A	449	THR
1	A	455	LEU
1	A	465	GLU
1	A	476	ARG
1	A	482	THR
1	A	487	GLU
1	A	497	LEU
1	A	498	ILE
1	A	505	PHE
2	B	11	LEU
2	B	35	SER
2	B	50	TYR
2	B	66	ARG
2	B	74	SER
2	B	95	CYS
2	B	97	ARG
2	B	99	THR
2	B	143	SER
2	B	152	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	156	THR
2	B	157	CYS
2	B	167	LEU
2	B	187	ASN
2	B	199	SER
2	B	208	THR
2	B	212	LEU
2	B	213	GLN
2	B	215	GLU
1	C	191	ASN
1	C	193	ILE
1	C	211	LYS
1	C	230	ASP
1	C	302	LYS
1	C	333	LYS
1	C	343	LEU
1	C	366	LYS
1	C	391	GLU
1	C	423	ARG
1	C	449	THR
1	C	455	LEU
1	C	465	GLU
1	C	476	ARG
1	C	482	THR
1	C	487	GLU
1	C	496	HIS
1	C	501	LEU
1	C	505	PHE
2	D	11	LEU
2	D	21	THR
2	D	35	SER
2	D	50	TYR
2	D	57	THR
2	D	66	ARG
2	D	74	SER
2	D	79	SER
2	D	95	CYS
2	D	97	ARG
2	D	107	ASP
2	D	116	THR
2	D	135	ASP
2	D	140	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	152	ARG
2	D	156	THR
2	D	157	CYS
2	D	167	LEU
2	D	173	LYS
2	D	179	LYS
2	D	189	GLU
2	D	194	SER
2	D	195	ARG
2	D	208	THR
2	D	212	LEU
2	D	215	GLU
2	D	239	GLU
1	E	191	ASN
1	E	196	LYS
1	E	230	ASP
1	E	333	LYS
1	E	344	SER
1	E	357	ARG
1	E	397	LEU
1	E	449	THR
1	E	455	LEU
1	E	465	GLU
1	E	476	ARG
1	E	482	THR
1	E	487	GLU
1	E	505	PHE
2	F	11	LEU
2	F	21	THR
2	F	35	SER
2	F	50	TYR
2	F	74	SER
2	F	79	SER
2	F	95	CYS
2	F	97	ARG
2	F	107	ASP
2	F	135	ASP
2	F	136	ILE
2	F	140	GLN
2	F	143	SER
2	F	152	ARG
2	F	157	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	163	ILE
2	F	167	LEU
2	F	173	LYS
2	F	179	LYS
2	F	189	GLU
2	F	199	SER
2	F	208	THR
2	F	212	LEU
2	F	213	GLN
2	F	215	GLU
2	F	228	LEU
2	F	241	LYS
1	G	191	ASN
1	G	196	LYS
1	G	230	ASP
1	G	333	LYS
1	G	345	CYS
1	G	357	ARG
1	G	385	ASN
1	G	397	LEU
1	G	449	THR
1	G	455	LEU
1	G	465	GLU
1	G	476	ARG
1	G	482	THR
1	G	487	GLU
2	H	5	GLN
2	H	11	LEU
2	H	21	THR
2	H	35	SER
2	H	50	TYR
2	H	66	ARG
2	H	74	SER
2	H	79	SER
2	H	95	CYS
2	H	97	ARG
2	H	105	TYR
2	H	137	GLN
2	H	143	SER
2	H	152	ARG
2	H	156	THR
2	H	157	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	167	LEU
2	H	179	LYS
2	H	180	VAL
2	H	189	GLU
2	H	199	SER
2	H	208	THR
2	H	212	LEU
2	H	213	GLN
2	H	215	GLU
1	I	191	ASN
1	I	200	TYR
1	I	230	ASP
1	I	333	LYS
1	I	343	LEU
1	I	345	CYS
1	I	357	ARG
1	I	393	LEU
1	I	449	THR
1	I	455	LEU
1	I	465	GLU
1	I	476	ARG
1	I	482	THR
1	I	487	GLU
1	I	494	PHE
1	I	497	LEU
2	J	11	LEU
2	J	21	THR
2	J	35	SER
2	J	50	TYR
2	J	66	ARG
2	J	74	SER
2	J	79	SER
2	J	95	CYS
2	J	116	THR
2	J	152	ARG
2	J	156	THR
2	J	157	CYS
2	J	167	LEU
2	J	189	GLU
2	J	199	SER
2	J	208	THR
2	J	212	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	J	228	LEU
1	K	203	TYR
1	K	230	ASP
1	K	303	MET
1	K	304	MET
1	K	333	LYS
1	K	343	LEU
1	K	345	CYS
1	K	396	ASN
1	K	397	LEU
1	K	449	THR
1	K	455	LEU
1	K	465	GLU
1	K	476	ARG
1	K	482	THR
1	K	487	GLU
1	K	494	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	A	492	ASN
1	A	495	HIS
1	G	165	GLN
1	G	388	GLN
1	I	165	GLN
1	K	165	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

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	288/338 (85%)	0.38	9 (3%)	51	33	73, 111, 167, 193	0
1	C	288/338 (85%)	0.42	17 (5%)	29	17	78, 119, 171, 190	0
1	E	287/338 (84%)	0.47	15 (5%)	34	20	79, 123, 185, 212	0
1	G	286/338 (84%)	0.36	5 (1%)	69	51	72, 110, 184, 218	0
1	I	288/338 (85%)	0.60	23 (7%)	20	11	149, 177, 208, 225	0
1	K	288/338 (85%)	0.86	30 (10%)	13	8	173, 202, 226, 235	0
2	B	223/250 (89%)	0.16	7 (3%)	51	33	64, 103, 135, 149	1 (0%)
2	D	226/250 (90%)	0.18	9 (3%)	43	26	67, 103, 125, 136	1 (0%)
2	F	226/250 (90%)	0.10	4 (1%)	67	50	64, 103, 126, 138	1 (0%)
2	H	226/250 (90%)	0.21	5 (2%)	62	44	65, 104, 133, 145	1 (0%)
2	J	222/250 (88%)	0.80	27 (12%)	10	6	139, 207, 223, 227	1 (0%)
All	All	2848/3278 (86%)	0.43	151 (5%)	33	20	64, 124, 214, 235	5 (0%)

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	158	ALA	5.9
1	K	336	GLY	5.8
2	J	41	PRO	5.5
2	F	118	SER	5.5
1	E	158	ALA	5.1
1	I	438	ILE	5.0
1	A	404	TYR	4.6
1	I	158	ALA	4.5
1	K	390	SER	4.4
1	I	405	ILE	4.0
1	G	404	TYR	4.0
1	G	158	ALA	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	J	149	LEU	3.9
1	K	158	ALA	3.8
2	H	118	SER	3.8
2	F	229	PRO	3.8
2	J	145	LEU	3.7
1	K	404	TYR	3.7
1	C	390	SER	3.6
1	I	338	ASN	3.6
1	E	163	ILE	3.6
1	K	328	ILE	3.6
1	I	202	LYS	3.6
1	A	158	ALA	3.5
1	C	238	LEU	3.5
1	K	405	ILE	3.5
1	K	394	LEU	3.5
1	K	339	LEU	3.4
1	K	456	LEU	3.4
1	C	404	TYR	3.4
1	I	463	SER	3.4
2	J	238	LEU	3.4
1	K	332	MET	3.4
1	K	210	ILE	3.2
1	K	315	ILE	3.1
2	D	229	PRO	3.0
2	B	190	THR	3.0
2	J	62	SER	3.0
1	K	191	ASN	3.0
1	I	404	TYR	2.9
1	A	482	THR	2.9
1	E	495	HIS	2.9
2	H	229	PRO	2.9
2	J	115	VAL	2.9
2	J	153	VAL	2.9
1	K	356	ILE	2.9
2	J	155	ILE	2.9
2	D	10	GLY	2.9
1	I	456	LEU	2.9
1	E	302	LYS	2.8
2	J	217	ILE	2.8
2	J	35	SER	2.8
1	K	182	LEU	2.8
2	J	117	VAL	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	405	ILE	2.8
2	B	147	ALA	2.7
2	D	228	LEU	2.7
1	K	500	VAL	2.7
2	B	136	ILE	2.7
1	E	468	LEU	2.7
1	K	200	TYR	2.7
2	J	70	SER	2.7
1	A	163	ILE	2.7
1	E	177	PRO	2.6
1	I	339	LEU	2.6
2	J	147	ALA	2.6
1	I	358	TYR	2.6
2	J	116	THR	2.6
1	E	499	TYR	2.6
1	K	329	CYS	2.6
1	I	442	ILE	2.6
2	J	212	LEU	2.6
1	A	189	SER	2.6
1	G	228	LYS	2.6
2	J	37	ILE	2.6
1	K	393	LEU	2.6
1	K	397	LEU	2.6
1	I	214	ASN	2.6
1	I	459	ILE	2.5
1	E	404	TYR	2.5
1	I	395	THR	2.5
2	B	98	SER	2.5
2	F	116	THR	2.5
1	K	334	ASN	2.5
1	I	501	LEU	2.5
2	D	193	PRO	2.5
2	B	91	ALA	2.5
2	J	88	ALA	2.5
1	I	401	MET	2.5
2	J	139	THR	2.4
2	D	1	GLN	2.4
1	I	390	SER	2.4
1	E	213	ILE	2.4
1	E	416	GLU	2.4
1	E	446	ILE	2.4
2	J	228	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	78	PHE	2.4
2	B	229	PRO	2.4
1	A	240	HIS	2.4
1	C	401	MET	2.4
2	J	220	TYR	2.4
2	J	179	LYS	2.4
2	D	207	PHE	2.4
2	D	206	THR	2.4
2	J	199	SER	2.4
1	C	505	PHE	2.4
1	E	240	HIS	2.4
1	K	343	LEU	2.3
1	C	386	ILE	2.3
1	G	504	LYS	2.3
2	F	228	LEU	2.3
2	J	63	LEU	2.3
2	D	199	SER	2.3
1	K	401	MET	2.3
1	C	362	GLU	2.3
1	I	171	LEU	2.3
1	A	161	ILE	2.3
2	J	14	PRO	2.3
1	C	495	HIS	2.2
1	K	407	ILE	2.2
1	C	307	TYR	2.2
1	E	328	ILE	2.2
1	G	348	ASN	2.2
1	E	303	MET	2.2
1	E	444	LEU	2.2
1	C	215	GLU	2.2
1	C	481	ASN	2.2
1	I	228	LYS	2.2
2	B	173	LYS	2.2
1	K	176	ILE	2.2
1	K	366	LYS	2.2
1	I	199	THR	2.2
1	K	231	LEU	2.2
1	C	393	LEU	2.2
2	J	18	LEU	2.2
2	J	73	THR	2.2
1	I	208	ALA	2.1
2	H	147	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	447	TRP	2.1
2	J	36	TRP	2.1
1	K	213	ILE	2.1
2	H	155	ILE	2.1
1	C	302	LYS	2.1
1	K	337	THR	2.1
1	K	410	ILE	2.1
1	C	240	HIS	2.1
1	I	240	HIS	2.1
1	C	483	PHE	2.1
2	H	181	LEU	2.1
1	I	489	HIS	2.0
1	C	355	GLY	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.