Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2023 – 06:54 AM EDT

PDB ID	:	6BPE
Title	:	Plasmodium vivax reticulocyte binding protein 2b (PvRBP2b) bound to monoclonal antibody 6H1
Authors	:	Gruszczyk, J.; Chan, L.J.; Tham, W.H.
Deposited on	:	2017-11-22
Resolution	:	3.34 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:

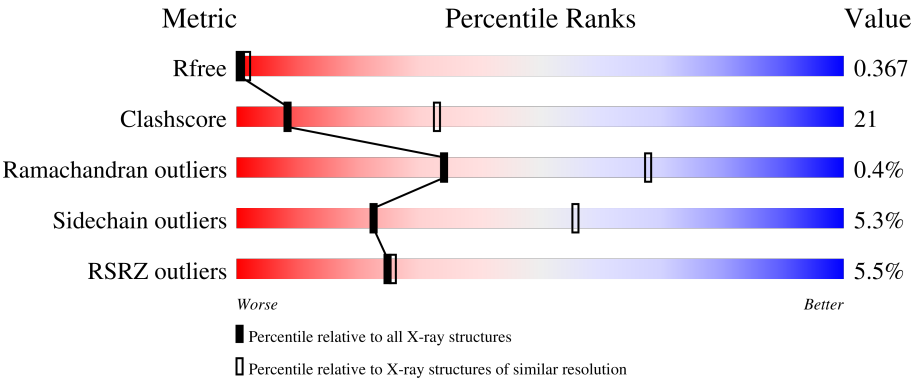
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.34 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}	130704	1060 (3.38-3.30)
Clashscore	141614	1111 (3.38-3.30)
Ramachandran outliers	138981	1090 (3.38-3.30)
Sidechain outliers	138945	1089 (3.38-3.30)
RSRZ outliers	127900	1028 (3.38-3.30)

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 <=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	307	3% 64% 33%
1	D	307	5% 66% 31%
1	G	307	2% 58% 36%
1	J	307	4% 50% 44%
2	B	254	7% 43% 37% 18%

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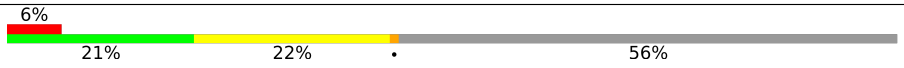
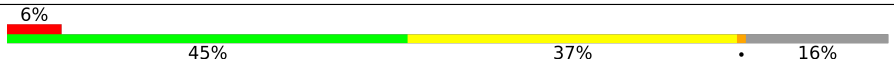
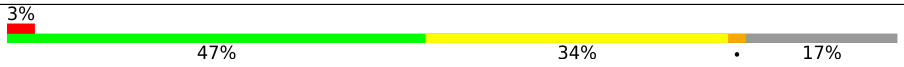
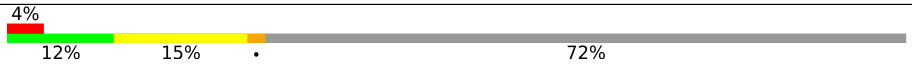
Mol	Chain	Length	Quality of chain
2	E	254	
2	H	254	
3	C	238	
3	F	238	
3	I	238	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 17777 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 2, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	0	0
			2518	1612	430	467	9			
1	D	302	Total	C	N	O	S	0	0	0
			2544	1627	436	472	9			
1	G	302	Total	C	N	O	S	0	0	0
			2543	1627	436	471	9			
1	J	297	Total	C	N	O	S	0	0	0
			2500	1602	428	461	9			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	164	GLY	-	expression tag	UNP A5K736
A	165	ALA	-	expression tag	UNP A5K736
A	166	MET	-	expression tag	UNP A5K736
A	167	GLY	-	expression tag	UNP A5K736
A	168	SER	-	expression tag	UNP A5K736
D	164	GLY	-	expression tag	UNP A5K736
D	165	ALA	-	expression tag	UNP A5K736
D	166	MET	-	expression tag	UNP A5K736
D	167	GLY	-	expression tag	UNP A5K736
D	168	SER	-	expression tag	UNP A5K736
G	164	GLY	-	expression tag	UNP A5K736
G	165	ALA	-	expression tag	UNP A5K736
G	166	MET	-	expression tag	UNP A5K736
G	167	GLY	-	expression tag	UNP A5K736
G	168	SER	-	expression tag	UNP A5K736
J	164	GLY	-	expression tag	UNP A5K736
J	165	ALA	-	expression tag	UNP A5K736
J	166	MET	-	expression tag	UNP A5K736
J	167	GLY	-	expression tag	UNP A5K736
J	168	SER	-	expression tag	UNP A5K736

- Molecule 2 is a protein called Monoclonal antibody 6H1 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	209	Total	C	N	O	S	0	0	0
			1594	1013	252	321	8			
2	E	208	Total	C	N	O	S	0	0	0
			1590	1011	254	318	7			
2	H	113	Total	C	N	O	S	0	0	0
			885	560	140	180	5			

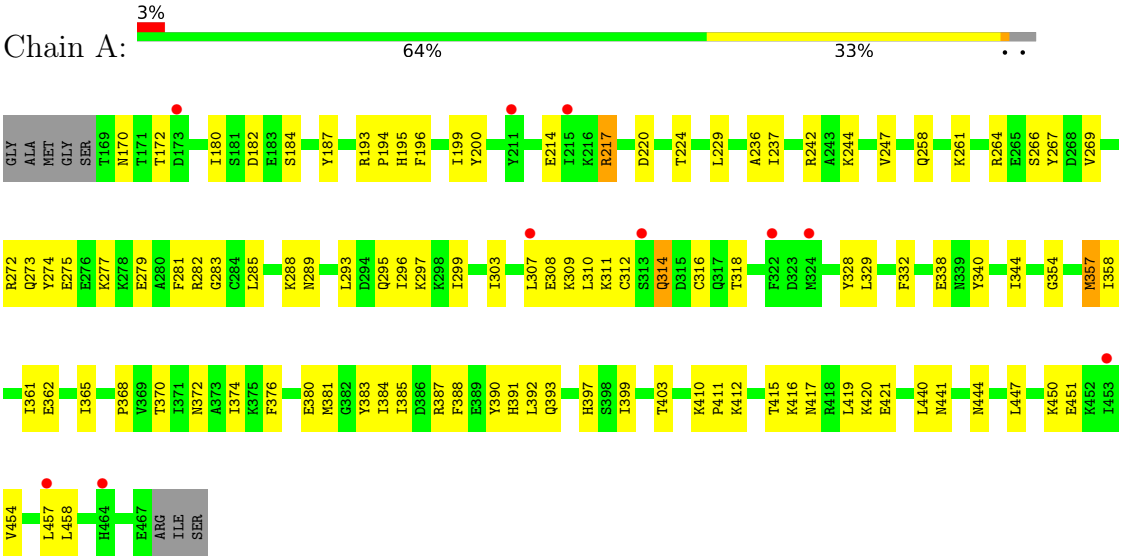
- Molecule 3 is a protein called Monoclonal antibody 6H1 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	199	Total	C	N	O	S	0	0	0
			1539	960	258	314	7			
3	F	198	Total	C	N	O	S	0	0	0
			1535	962	255	311	7			
3	I	67	Total	C	N	O	S	0	0	0
			529	334	88	105	2			

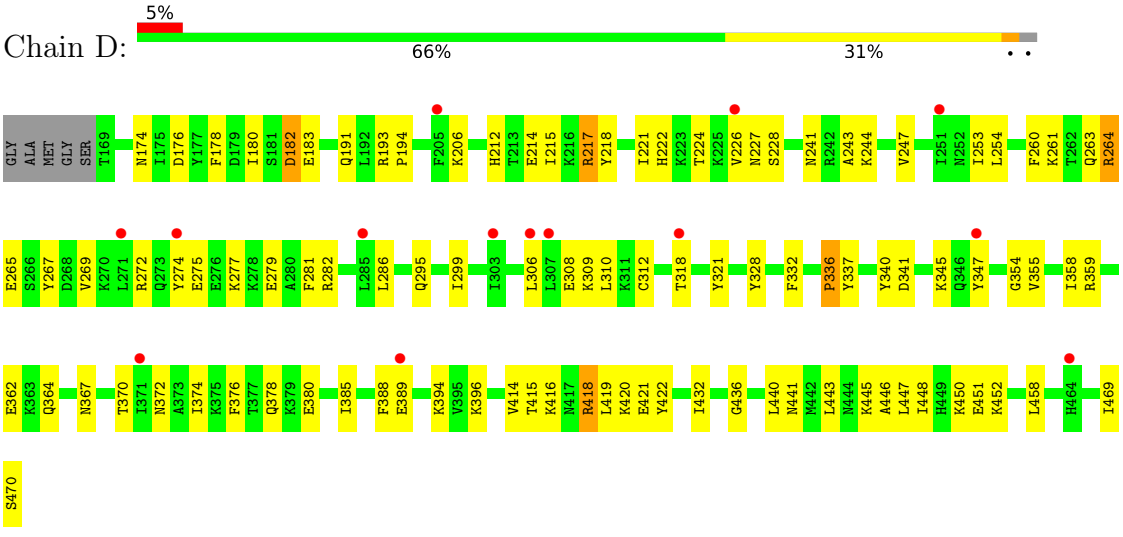
3 Residue-property plots (i)

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.

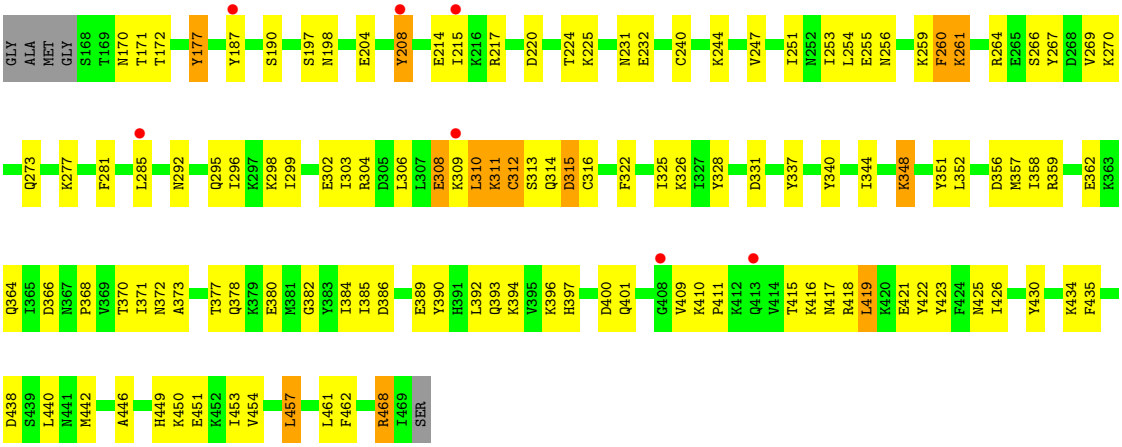
• Molecule 1: Reticulocyte binding protein 2, putative



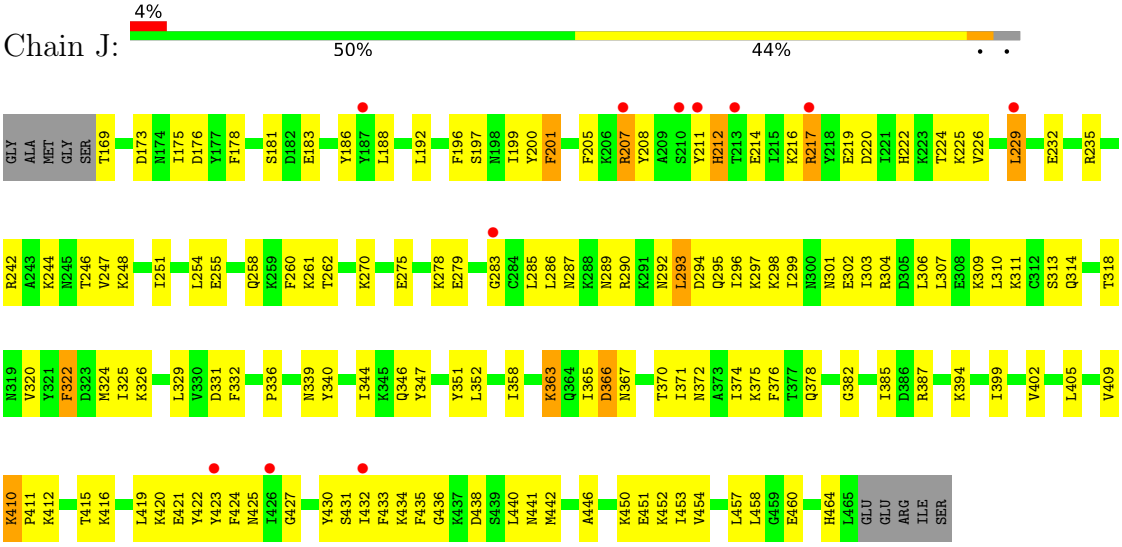
• Molecule 1: Reticulocyte binding protein 2, putative



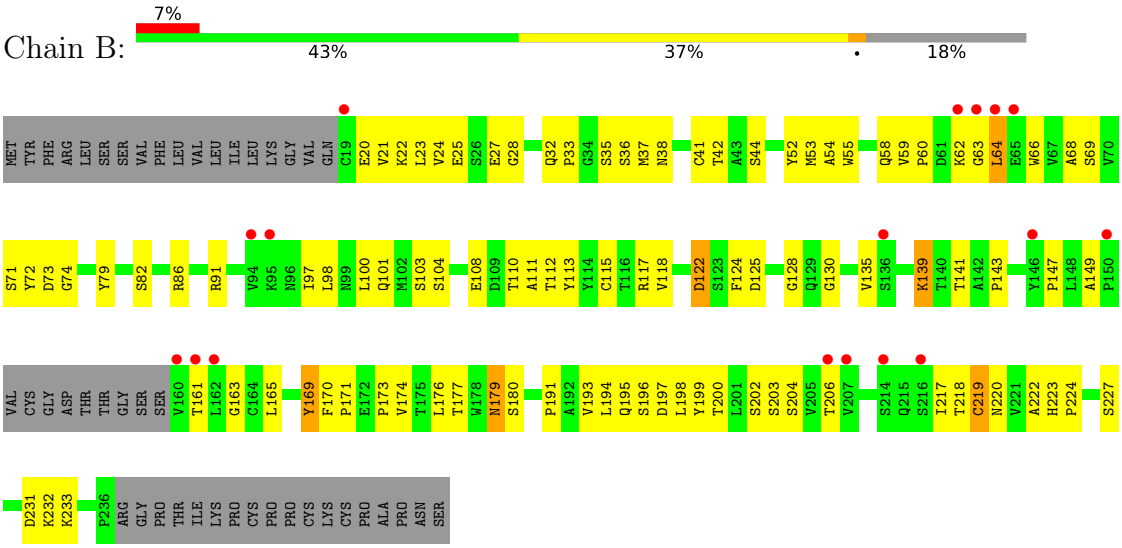
• Molecule 1: Reticulocyte binding protein 2, putative



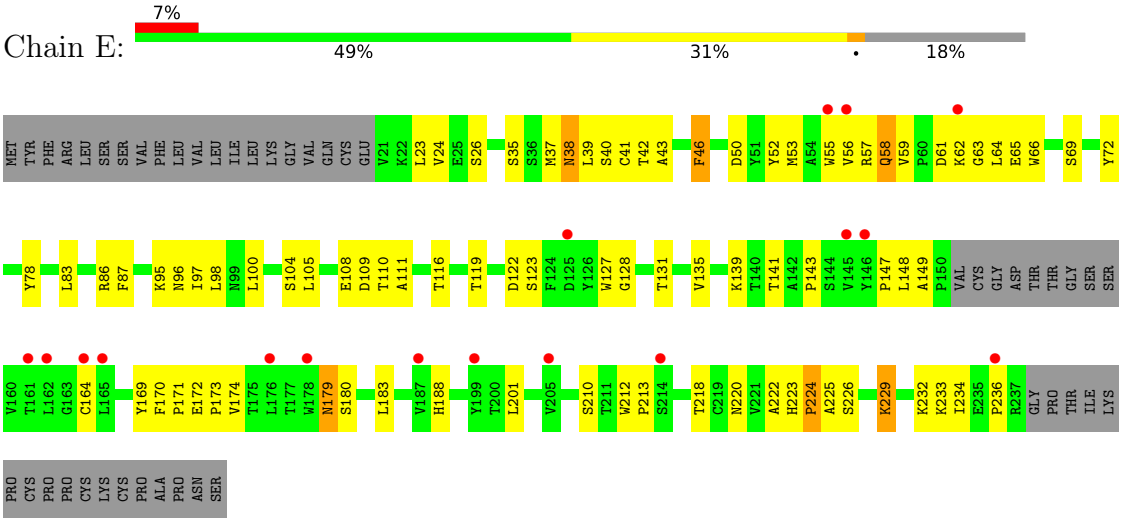
• Molecule 1: Reticulocyte binding protein 2, putative



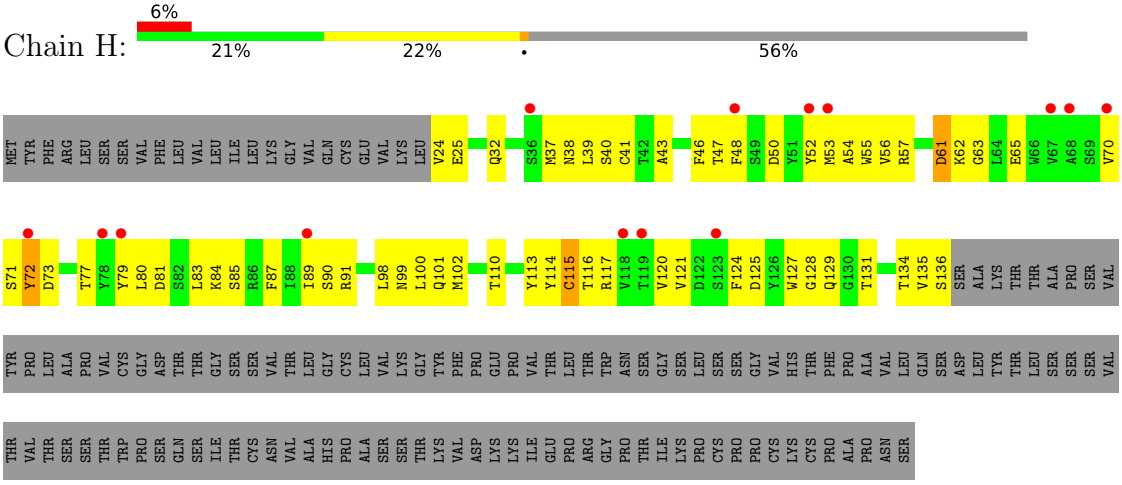
• Molecule 2: Monoclonal antibody 6H1 Fab heavy chain



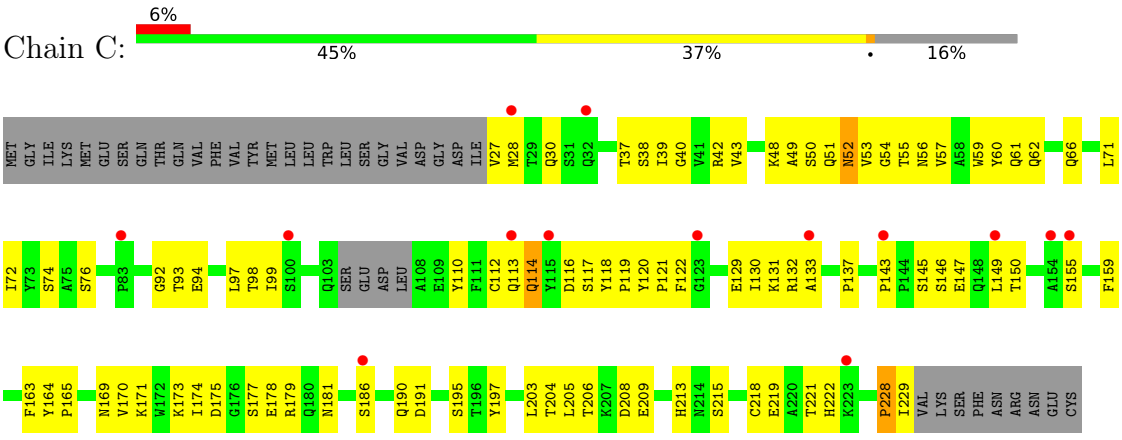
• Molecule 2: Monoclonal antibody 6H1 Fab heavy chain



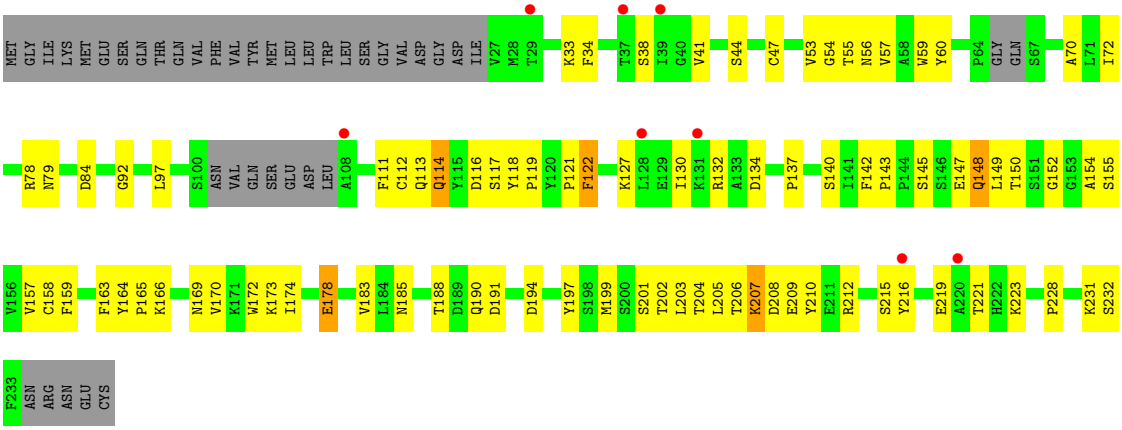
• Molecule 2: Monoclonal antibody 6H1 Fab heavy chain



• Molecule 3: Monoclonal antibody 6H1 Fab light chain

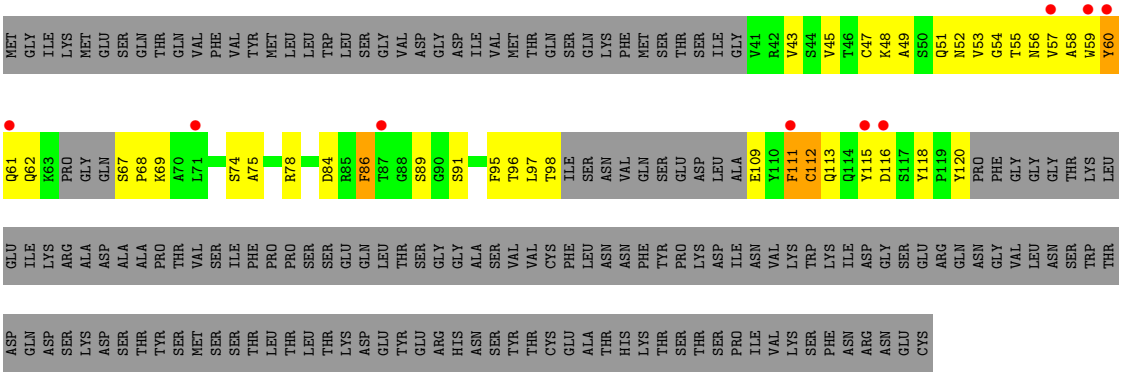


• Molecule 3: Monoclonal antibody 6H1 Fab light chain



• Molecule 3: Monoclonal antibody 6H1 Fab light chain

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	106.60Å 123.48Å 143.28Å 90.00° 105.25° 90.00°	Depositor
Resolution (Å)	73.75 – 3.34 75.49 – 3.34	Depositor EDS
% Data completeness (in resolution range)	99.2 (73.75-3.34) 99.4 (75.49-3.34)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.82 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.318 , 0.367 0.318 , 0.367	Depositor DCC
R_{free} test set	1068 reflections (2.06%)	wwPDB-VP
Wilson B-factor (Å^2)	75.2	Xtriage
Anisotropy	0.681	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 45.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.81	EDS
Total number of atoms	17777	wwPDB-VP
Average B, all atoms (Å^2)	86.0	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 30.93 % 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 1.2039e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.25	0/2567	0.36	0/3444
1	D	0.24	0/2593	0.38	0/3477
1	G	0.26	0/2592	0.43	0/3477
1	J	0.27	0/2549	0.46	0/3420
2	B	0.27	0/1632	0.53	0/2231
2	E	0.27	0/1628	0.51	0/2225
2	H	0.29	0/904	0.51	0/1229
3	C	0.26	0/1574	0.51	0/2136
3	F	0.29	0/1570	0.51	0/2128
3	I	0.35	0/541	0.62	0/732
All	All	0.27	0/18150	0.46	0/24499

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

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	2518	0	2523	72	0
1	D	2544	0	2552	68	0
1	G	2543	0	2552	104	0
1	J	2500	0	2511	107	0
2	B	1594	0	1555	80	0
2	E	1590	0	1557	75	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	885	0	843	60	0
3	C	1539	0	1465	70	0
3	F	1535	0	1466	69	0
3	I	529	0	491	68	0
All	All	17777	0	17515	736	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 21.

All (736) 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)
3:I:57:VAL:CG2	3:I:59:TRP:CH2	1.76	1.62
3:I:57:VAL:HG21	3:I:59:TRP:CH2	1.37	1.49
3:I:57:VAL:HG23	3:I:59:TRP:CZ3	1.48	1.44
3:I:53:VAL:HG21	3:I:116:ASP:CG	1.48	1.33
2:E:56:VAL:HG23	2:E:65:GLU:O	1.24	1.30
3:I:53:VAL:HG21	3:I:116:ASP:OD1	1.33	1.29
3:I:59:TRP:CD1	3:I:112:CYS:HB3	1.67	1.28
3:I:57:VAL:HG21	3:I:59:TRP:CZ2	1.67	1.27
3:C:219:GLU:OE2	3:C:228:PRO:HB2	1.25	1.26
3:C:219:GLU:OE2	3:C:228:PRO:CB	1.83	1.25
2:E:56:VAL:CG2	2:E:65:GLU:O	1.93	1.15
3:I:57:VAL:HG23	3:I:59:TRP:CH2	1.56	1.12
3:I:52:ASN:ND2	3:I:54:GLY:O	1.92	1.01
3:I:59:TRP:CD1	3:I:112:CYS:CB	2.44	1.00
2:E:64:LEU:O	3:F:122:PHE:CE1	2.09	0.99
3:I:53:VAL:CG2	3:I:116:ASP:CG	2.33	0.97
3:F:113:GLN:HG3	3:F:122:PHE:HD2	1.33	0.94
2:H:114:TYR:HH	3:I:67:SER:N	1.64	0.93
3:C:28:MET:HB2	3:C:50:SER:H	1.32	0.92
2:B:62:LYS:HB3	2:B:63:GLY:HA2	1.53	0.91
1:G:311:LYS:CB	3:I:53:VAL:O	2.20	0.90
3:I:58:ALA:H	3:I:115:TYR:HE2	1.16	0.90
2:E:58:GLN:HE21	2:E:62:LYS:HG3	1.37	0.89
3:C:53:VAL:HG11	3:C:114:GLN:HG3	1.56	0.88
2:E:179:ASN:HD21	2:E:183:LEU:HD13	1.39	0.88
3:I:59:TRP:HD1	3:I:112:CYS:HB3	1.32	0.87
3:I:57:VAL:CG2	3:I:59:TRP:HH2	1.77	0.87
3:I:59:TRP:HZ3	3:I:75:ALA:HB2	1.39	0.86
3:I:57:VAL:CG2	3:I:59:TRP:CZ2	2.42	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:PHE:HB2	2:B:198:LEU:HD21	1.58	0.83
2:B:177:THR:HB	2:B:220:ASN:HB2	1.60	0.83
1:D:418:ARG:NH2	1:D:421:GLU:OE1	2.11	0.82
1:J:318:THR:H	1:J:412:LYS:HG3	1.45	0.81
1:J:205:PHE:HA	1:J:208:TYR:HD2	1.46	0.81
1:G:311:LYS:HB3	3:I:53:VAL:O	1.79	0.80
2:B:179:ASN:HA	2:B:217:ILE:HG21	1.64	0.80
1:G:311:LYS:HB3	3:I:53:VAL:C	2.01	0.79
3:C:137:PRO:HD3	3:C:222:HIS:HD2	1.47	0.79
3:I:55:THR:HG21	3:I:91:SER:HA	1.65	0.79
3:C:219:GLU:CD	3:C:228:PRO:CB	2.51	0.79
2:E:110:THR:HG23	2:E:135:VAL:H	1.47	0.79
3:F:137:PRO:HB3	3:F:163:PHE:HB3	1.64	0.78
2:E:86:ARG:NH2	2:E:109:ASP:OD2	2.17	0.77
2:H:84:LYS:NZ	2:H:85:SER:H	1.82	0.77
1:J:290:ARG:HD2	1:J:293:LEU:HD21	1.66	0.77
1:J:421:GLU:O	1:J:425:ASN:N	2.18	0.77
1:D:247:VAL:HG22	1:D:277:LYS:HB3	1.66	0.76
3:I:59:TRP:CZ2	3:I:95:PHE:HB3	2.20	0.76
3:C:206:THR:OG1	3:C:208:ASP:OD1	2.04	0.75
1:J:214:GLU:HG3	1:J:311:LYS:H	1.50	0.75
1:G:224:THR:HG21	2:H:73:ASP:OD2	1.87	0.75
3:F:172:TRP:HE1	3:F:201:SER:HB3	1.50	0.74
3:C:205:LEU:HD11	3:C:209:GLU:HB2	1.66	0.74
1:D:367:ASN:OD1	1:D:370:THR:OG1	2.05	0.74
2:E:58:GLN:NE2	2:E:59:VAL:O	2.20	0.74
2:E:180:SER:H	2:E:220:ASN:HD21	1.35	0.74
2:B:27:GLU:OE2	2:B:27:GLU:N	2.21	0.74
3:F:209:GLU:HA	3:F:212:ARG:HD3	1.70	0.73
3:C:129:GLU:OE2	3:C:197:TYR:OH	2.07	0.73
2:H:55:TRP:NE1	2:H:115:CYS:SG	2.62	0.73
1:A:217:ARG:NH2	2:B:72:TYR:OH	2.20	0.73
2:E:147:PRO:O	3:F:145:SER:OG	2.06	0.72
2:B:117:ARG:NE	2:B:125:ASP:OD2	2.20	0.72
2:B:110:THR:HG22	2:B:135:VAL:H	1.54	0.72
3:C:38:SER:HB3	3:C:131:LYS:HB2	1.72	0.72
3:I:43:VAL:HG23	3:I:98:THR:O	1.91	0.71
1:J:217:ARG:HH22	1:J:309:LYS:HD3	1.53	0.71
3:I:53:VAL:CG2	3:I:116:ASP:OD1	2.27	0.71
1:A:172:THR:HG21	1:A:450:LYS:HE2	1.73	0.70
3:F:174:ILE:O	3:F:174:ILE:HD12	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:311:LYS:HB2	3:I:53:VAL:O	1.91	0.70
3:C:219:GLU:OE2	3:C:228:PRO:CG	2.38	0.70
2:E:43:ALA:HB1	2:E:46:PHE:HE1	1.57	0.70
2:E:64:LEU:C	3:F:122:PHE:CZ	2.37	0.70
2:B:82:SER:O	2:B:86:ARG:NH2	2.24	0.70
1:D:178:PHE:O	1:D:191:GLN:NE2	2.21	0.70
3:F:78:ARG:NH2	3:F:84:ASP:OD1	2.26	0.69
3:I:58:ALA:HB3	3:I:115:TYR:CZ	2.28	0.69
2:B:25:GLU:HG2	2:B:55:TRP:HH2	1.55	0.69
2:B:220:ASN:HA	2:B:231:ASP:OD1	1.93	0.69
1:D:347:TYR:OH	1:D:447:LEU:O	2.10	0.68
1:G:311:LYS:HD3	3:I:53:VAL:O	1.93	0.68
2:H:53:MET:HB3	2:H:98:LEU:HD22	1.76	0.68
3:C:219:GLU:CD	3:C:228:PRO:HB2	2.10	0.68
2:B:191:PRO:HG2	3:C:186:SER:HB2	1.75	0.68
2:E:39:LEU:HD22	2:E:131:THR:HG21	1.76	0.68
1:G:267:TYR:HB3	1:G:372:ASN:HD22	1.59	0.68
1:J:344:ILE:HD11	1:J:385:ILE:HG23	1.75	0.68
1:J:454:VAL:O	1:J:458:LEU:N	2.23	0.68
2:H:84:LYS:HZ1	2:H:85:SER:H	1.41	0.67
1:J:205:PHE:HA	1:J:208:TYR:CD2	2.29	0.67
1:A:247:VAL:HG22	1:A:277:LYS:HB3	1.76	0.67
2:H:80:LEU:HB3	2:H:83:LEU:HB2	1.76	0.67
3:C:116:ASP:OD1	3:C:117:SER:OG	2.13	0.67
1:D:274:TYR:OH	1:D:380:GLU:OE2	2.13	0.67
1:J:176:ASP:HB3	1:J:442:MET:HE2	1.77	0.67
3:C:59:TRP:HB2	3:C:72:ILE:HB	1.76	0.67
2:E:56:VAL:HG22	2:E:65:GLU:O	1.95	0.66
1:A:357:MET:HG3	1:J:346:GLN:HG2	1.75	0.66
3:C:28:MET:SD	3:C:51:GLN:N	2.66	0.66
1:G:215:ILE:HG23	1:G:306:LEU:HD22	1.77	0.66
1:G:267:TYR:HB3	1:G:372:ASN:ND2	2.10	0.66
3:I:58:ALA:HB3	3:I:115:TYR:OH	1.95	0.66
3:I:60:TYR:OH	3:I:113:GLN:OE1	2.13	0.66
1:J:217:ARG:NE	1:J:306:LEU:HG	2.10	0.66
2:B:115:CYS:O	2:B:128:GLY:N	2.28	0.66
2:E:179:ASN:HB3	2:E:218:THR:H	1.60	0.66
3:F:174:ILE:HG22	3:F:216:TYR:HD1	1.61	0.66
1:G:419:LEU:HD12	1:G:423:TYR:CE2	2.30	0.66
2:E:83:LEU:O	2:E:83:LEU:HD12	1.95	0.65
1:G:416:LYS:HA	1:G:419:LEU:HD21	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:108:GLU:N	2:B:108:GLU:OE1	2.29	0.65
2:E:171:PRO:O	2:E:223:HIS:NE2	2.30	0.65
1:G:358:ILE:HD11	1:G:371:ILE:HG23	1.79	0.65
1:G:254:LEU:HD12	1:G:270:LYS:HD3	1.79	0.65
2:B:62:LYS:CB	2:B:63:GLY:HA2	2.23	0.65
3:I:57:VAL:CG2	3:I:59:TRP:CZ3	2.31	0.65
1:D:174:ASN:ND2	1:D:176:ASP:OD1	2.27	0.64
1:J:302:GLU:O	1:J:306:LEU:HD13	1.97	0.64
1:A:370:THR:HG22	1:A:457:LEU:HD21	1.80	0.64
3:C:56:ASN:ND2	3:C:116:ASP:OD2	2.31	0.64
2:E:218:THR:HG22	2:E:233:LYS:HA	1.78	0.64
3:C:60:TYR:OH	3:C:113:GLN:OE1	2.13	0.64
3:C:190:GLN:NE2	3:C:191:ASP:O	2.30	0.64
2:E:58:GLN:O	2:E:111:ALA:HB1	1.98	0.64
2:H:80:LEU:HD23	2:H:83:LEU:HD23	1.79	0.64
3:C:219:GLU:CD	3:C:228:PRO:HB3	2.17	0.64
3:C:62:GLN:NE2	3:C:66:GLN:O	2.31	0.63
2:B:25:GLU:HG2	2:B:55:TRP:CH2	2.32	0.63
3:F:147:GLU:N	3:F:147:GLU:OE1	2.31	0.63
2:B:41:CYS:HB3	2:B:98:LEU:HB3	1.79	0.63
2:E:147:PRO:HB3	2:E:234:ILE:HG12	1.81	0.63
3:F:172:TRP:CD1	3:F:183:VAL:HG21	2.34	0.63
1:A:309:LYS:NZ	2:B:122:ASP:OD1	2.31	0.63
2:B:58:GLN:HB3	2:B:112:THR:HB	1.79	0.63
3:F:206:THR:O	3:F:210:TYR:N	2.25	0.63
1:A:229:LEU:HD21	1:A:296:ILE:HG23	1.80	0.63
2:B:194:LEU:HA	2:B:199:TYR:HA	1.79	0.63
3:I:59:TRP:NE1	3:I:112:CYS:CB	2.62	0.63
3:C:30:GLN:HG2	3:C:49:ALA:HA	1.81	0.62
2:E:116:THR:HG22	2:E:127:TRP:HA	1.80	0.62
2:H:72:TYR:HA	2:H:91:ARG:NH1	2.14	0.62
2:E:38:ASN:HD22	2:E:39:LEU:H	1.47	0.62
2:E:55:TRP:HE1	2:E:98:LEU:HD22	1.64	0.62
3:C:114:GLN:HG2	3:C:116:ASP:H	1.64	0.62
2:E:26:SER:OG	2:E:40:SER:N	2.27	0.62
1:G:231:ASN:OD1	1:G:232:GLU:N	2.32	0.62
1:D:193:ARG:HG3	1:D:194:PRO:HA	1.81	0.62
2:E:86:ARG:HH21	2:E:105:LEU:HA	1.65	0.62
3:F:149:LEU:O	3:F:207:LYS:HD2	1.99	0.62
3:F:169:ASN:HB3	3:F:221:THR:HB	1.80	0.62
1:J:232:GLU:HA	1:J:235:ARG:HD3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:269:VAL:HG23	1:D:272:ARG:HH21	1.65	0.62
2:E:141:THR:O	2:E:226:SER:OG	2.18	0.62
1:G:295:GLN:O	1:G:299:ILE:HD12	1.98	0.62
3:C:113:GLN:HB2	3:C:122:PHE:HD1	1.65	0.62
1:G:309:LYS:HG3	2:H:121:VAL:HG12	1.81	0.61
1:A:440:LEU:O	1:A:444:ASN:ND2	2.32	0.61
1:J:421:GLU:HA	1:J:424:PHE:HB3	1.82	0.61
1:A:318:THR:OG1	1:A:411:PRO:O	2.14	0.61
3:I:59:TRP:HZ2	3:I:95:PHE:HB3	1.66	0.61
3:I:89:SER:O	3:I:96:THR:OG1	2.19	0.61
2:E:41:CYS:HB3	2:E:98:LEU:HB3	1.83	0.61
3:F:72:ILE:HD13	3:F:78:ARG:HB3	1.83	0.61
3:F:113:GLN:HG3	3:F:122:PHE:CD2	2.25	0.61
1:G:292:ASN:O	1:G:296:ILE:N	2.32	0.61
2:H:25:GLU:HG3	2:H:115:CYS:HB2	1.82	0.61
1:J:375:LYS:HA	1:J:378:GLN:HG3	1.83	0.61
1:J:214:GLU:HG3	1:J:310:LEU:HD12	1.81	0.60
1:J:382:GLY:HA2	1:J:385:ILE:HD12	1.83	0.60
3:C:137:PRO:HB3	3:C:163:PHE:HB3	1.83	0.60
3:I:59:TRP:NE1	3:I:112:CYS:HB3	2.16	0.60
2:B:35:SER:HB2	2:B:104:SER:H	1.66	0.60
2:E:95:LYS:HB3	2:E:97:ILE:HG12	1.84	0.60
1:G:386:ASP:HA	1:G:389:GLU:HB2	1.84	0.60
2:H:89:ILE:HA	2:H:100:LEU:HA	1.83	0.60
1:J:450:LYS:HA	1:J:453:ILE:HD12	1.84	0.60
2:H:73:ASP:N	2:H:73:ASP:OD1	2.34	0.60
2:E:105:LEU:HD12	2:E:105:LEU:H	1.65	0.60
1:G:204:GLU:OE1	1:G:328:TYR:OH	2.13	0.60
2:H:39:LEU:HD13	2:H:131:THR:HG21	1.84	0.60
1:A:417:ASN:HA	1:A:420:LYS:HD2	1.82	0.60
2:E:223:HIS:HD2	2:E:224:PRO:HD2	1.65	0.60
2:H:53:MET:HB3	2:H:98:LEU:CD2	2.32	0.60
3:F:185:ASN:HB3	3:F:201:SER:HA	1.83	0.59
3:F:55:THR:HG22	3:F:55:THR:O	2.02	0.59
1:G:220:ASP:O	1:G:224:THR:OG1	2.19	0.59
3:C:27:VAL:HG21	3:C:119:PRO:HD2	1.84	0.59
2:E:38:ASN:ND2	2:E:100:LEU:O	2.35	0.59
1:D:337:TYR:CE2	1:D:396:LYS:HB2	2.37	0.59
2:H:32:GLN:NE2	2:H:136:SER:O	2.36	0.59
2:B:54:ALA:HB2	2:B:69:SER:HB3	1.84	0.59
1:J:374:ILE:HA	1:J:457:LEU:HD13	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ARG:HG3	1:A:194:PRO:HA	1.83	0.59
1:G:425:ASN:OD1	1:G:426:ILE:N	2.36	0.59
3:C:213:HIS:ND1	3:C:215:SER:O	2.36	0.58
2:E:38:ASN:HD22	2:E:39:LEU:N	2.00	0.58
1:G:348:LYS:O	1:G:352:LEU:HG	2.03	0.58
1:J:200:TYR:OH	1:J:438:ASP:OD2	2.20	0.58
2:B:24:VAL:HG12	2:B:42:THR:HB	1.84	0.58
2:E:24:VAL:HG22	2:E:42:THR:HB	1.85	0.58
1:J:293:LEU:HA	1:J:296:ILE:HD12	1.85	0.58
1:J:365:ILE:HD12	1:J:366:ASP:H	1.69	0.58
2:E:37:MET:SD	2:E:38:ASN:N	2.77	0.58
2:H:62:LYS:N	2:H:63:GLY:HA2	2.19	0.58
2:B:71:SER:O	2:B:91:ARG:NH1	2.36	0.57
3:C:164:TYR:CD1	3:C:165:PRO:HA	2.39	0.57
3:F:173:LYS:HB3	3:F:178:GLU:HB3	1.86	0.57
1:J:169:THR:HG21	1:J:452:LYS:HB3	1.85	0.57
1:J:254:LEU:HD11	1:J:270:LYS:HB3	1.86	0.57
1:G:409:VAL:HG13	1:G:411:PRO:HD3	1.86	0.57
1:G:311:LYS:CD	3:I:53:VAL:O	2.52	0.57
1:A:374:ILE:HD12	1:A:454:VAL:HG23	1.86	0.57
3:I:59:TRP:CZ3	3:I:75:ALA:HB2	2.29	0.57
2:E:65:GLU:N	3:F:122:PHE:CZ	2.72	0.57
2:H:117:ARG:O	2:H:125:ASP:N	2.34	0.57
1:J:415:THR:O	1:J:419:LEU:N	2.38	0.57
1:D:310:LEU:O	1:D:416:LYS:NZ	2.34	0.57
1:A:267:TYR:CZ	1:A:372:ASN:HB3	2.39	0.57
1:D:469:ILE:HD12	1:D:470:SER:N	2.19	0.57
2:E:83:LEU:HD22	2:E:87:PHE:CD1	2.40	0.57
3:F:155:SER:HA	3:F:204:THR:HA	1.87	0.57
3:F:174:ILE:HG22	3:F:216:TYR:CD1	2.39	0.57
2:B:35:SER:HB2	2:B:104:SER:N	2.19	0.57
3:F:158:CYS:HB2	3:F:172:TRP:CZ2	2.40	0.56
2:H:48:PHE:HB3	2:H:91:ARG:HH22	1.70	0.56
1:J:196:PHE:HB2	1:J:199:ILE:HG12	1.86	0.56
2:H:110:THR:OG1	2:H:134:THR:HA	2.04	0.56
1:J:247:VAL:O	1:J:251:ILE:HG13	2.05	0.56
2:E:43:ALA:HB1	2:E:46:PHE:CE1	2.41	0.56
2:H:87:PHE:HB3	2:H:102:MET:HA	1.86	0.56
3:I:86:PHE:CZ	3:I:98:THR:O	2.59	0.56
1:A:180:ILE:HD12	1:A:282:ARG:HB3	1.88	0.56
3:C:132:ARG:HG3	3:C:133:ALA:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:113:GLN:HE21	3:I:120:TYR:HB3	1.70	0.56
1:D:355:VAL:HG13	1:D:359:ARG:HH22	1.71	0.56
3:F:116:ASP:OD1	3:F:117:SER:OG	2.23	0.56
3:I:61:GLN:HG2	3:I:109:GLU:O	2.04	0.56
3:F:215:SER:HA	3:F:232:SER:HA	1.87	0.56
1:D:370:THR:O	1:D:374:ILE:HG13	2.05	0.56
1:D:469:ILE:HD12	1:D:470:SER:H	1.70	0.56
3:F:173:LYS:HA	3:F:178:GLU:HB3	1.87	0.56
2:H:57:ARG:NH1	2:H:65:GLU:OE1	2.39	0.56
2:E:58:GLN:NE2	2:E:62:LYS:HG3	2.14	0.56
1:G:309:LYS:HD2	2:H:121:VAL:HA	1.86	0.56
1:J:201:PHE:CE2	1:J:431:SER:HB2	2.41	0.56
3:C:59:TRP:CD2	3:C:97:LEU:HD12	2.42	0.55
1:J:225:LYS:O	1:J:229:LEU:HD23	2.07	0.55
1:D:341:ASP:O	1:D:345:LYS:HG2	2.06	0.55
1:G:370:THR:HG21	1:G:461:LEU:HB2	1.88	0.55
2:H:24:VAL:N	2:H:25:GLU:OE1	2.39	0.55
1:A:220:ASP:O	1:A:224:THR:OG1	2.23	0.55
1:D:308:GLU:OE1	1:D:420:LYS:NZ	2.39	0.55
3:F:113:GLN:HA	3:F:122:PHE:HB3	1.88	0.55
3:F:208:ASP:OD1	3:F:208:ASP:N	2.40	0.55
2:B:147:PRO:O	3:C:145:SER:OG	2.20	0.55
2:H:110:THR:HB	2:H:135:VAL:HG22	1.88	0.55
1:A:237:ILE:HD12	1:A:285:LEU:HD23	1.88	0.55
3:C:169:ASN:HB3	3:C:221:THR:HB	1.89	0.55
1:D:440:LEU:HA	1:D:443:LEU:HD12	1.88	0.55
1:A:332:PHE:CD1	1:A:399:ILE:HG22	2.41	0.55
3:F:53:VAL:HG12	3:F:56:ASN:HB2	1.89	0.55
2:H:87:PHE:HB2	2:H:101:GLN:O	2.07	0.55
1:J:201:PHE:HE2	1:J:431:SER:HB2	1.72	0.55
3:C:146:SER:HA	3:C:149:LEU:HD21	1.89	0.54
3:F:119:PRO:HD2	3:F:121:PRO:HD3	1.90	0.54
1:G:225:LYS:HE3	2:H:50:ASP:HA	1.89	0.54
3:I:57:VAL:HG21	3:I:59:TRP:HH2	1.38	0.54
3:I:58:ALA:O	3:I:115:TYR:OH	2.16	0.54
1:J:295:GLN:HA	1:J:298:LYS:HD2	1.88	0.54
1:J:247:VAL:HG12	1:J:251:ILE:HD11	1.89	0.54
1:A:295:GLN:O	1:A:299:ILE:HG12	2.07	0.54
3:I:52:ASN:ND2	3:I:54:GLY:H	2.06	0.54
1:J:214:GLU:CG	1:J:311:LYS:H	2.19	0.54
1:A:358:ILE:HA	1:A:361:ILE:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:218:THR:HG22	2:B:219:CYS:O	2.08	0.54
3:F:140:SER:HB2	3:F:159:PHE:HB2	1.89	0.54
1:J:365:ILE:HD11	1:J:371:ILE:HD11	1.90	0.54
1:A:388:PHE:HE2	1:A:444:ASN:HB3	1.72	0.54
3:C:149:LEU:HD23	3:C:149:LEU:H	1.72	0.54
1:D:214:GLU:HG3	1:D:310:LEU:HA	1.90	0.54
1:G:419:LEU:HD12	1:G:423:TYR:HE2	1.73	0.54
1:J:325:ILE:O	1:J:329:LEU:HG	2.07	0.54
1:D:178:PHE:N	1:D:191:GLN:OE1	2.41	0.54
1:G:313:SER:O	1:G:314:GLN:HB2	2.08	0.54
2:B:66:TRP:HZ2	3:C:118:TYR:HD1	1.55	0.53
3:C:43:VAL:O	3:C:98:THR:HA	2.09	0.53
1:J:332:PHE:HE2	1:J:402:VAL:HG21	1.73	0.53
1:A:195:HIS:CD2	1:A:237:ILE:HG13	2.43	0.53
1:A:285:LEU:O	1:A:289:ASN:ND2	2.38	0.53
1:D:318:THR:HG22	1:D:419:LEU:HD13	1.90	0.53
2:E:108:GLU:N	2:E:108:GLU:OE1	2.41	0.53
3:F:130:ILE:HB	3:F:190:GLN:HE22	1.74	0.53
1:D:212:HIS:HB2	1:D:215:ILE:HG22	1.90	0.53
1:J:301:ASN:OD1	1:J:304:ARG:NH1	2.42	0.53
1:J:320:VAL:O	1:J:324:MET:N	2.41	0.53
1:D:218:TYR:HA	1:D:221:ILE:HD12	1.90	0.53
1:D:432:ILE:O	1:D:436:GLY:N	2.39	0.53
2:E:56:VAL:HG23	2:E:65:GLU:C	2.18	0.53
2:H:38:ASN:HB3	2:H:101:GLN:HG3	1.91	0.53
2:H:70:VAL:HG23	2:H:77:THR:HG22	1.91	0.53
1:A:374:ILE:HG12	1:A:457:LEU:HD22	1.91	0.53
1:D:318:THR:HB	1:D:321:TYR:HB3	1.91	0.53
1:D:340:TYR:HD2	1:D:388:PHE:HZ	1.57	0.52
2:B:143:PRO:HB3	2:B:169:TYR:HB3	1.91	0.52
1:A:332:PHE:HD1	1:A:399:ILE:HG22	1.73	0.52
1:G:322:PHE:O	1:G:326:LYS:HG2	2.09	0.52
1:G:356:ASP:OD1	1:G:356:ASP:N	2.39	0.52
2:H:87:PHE:CB	2:H:102:MET:HA	2.40	0.52
3:I:59:TRP:NE1	3:I:112:CYS:SG	2.83	0.52
1:J:226:VAL:HA	1:J:229:LEU:CD2	2.39	0.52
1:G:295:GLN:O	1:G:299:ILE:CD1	2.58	0.52
2:H:25:GLU:OE1	2:H:25:GLU:N	2.32	0.52
2:E:23:LEU:HD22	2:E:128:GLY:HA3	1.92	0.52
1:A:182:ASP:OD2	1:A:184:SER:OG	2.22	0.51
3:C:119:PRO:O	3:C:121:PRO:HD3	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:50:ASP:OD1	2:E:50:ASP:N	2.43	0.51
1:J:410:LYS:N	1:J:411:PRO:HD3	2.24	0.51
1:A:383:TYR:HD1	1:A:384:ILE:HD13	1.75	0.51
1:G:382:GLY:HA2	1:G:385:ILE:HD12	1.92	0.51
2:B:59:VAL:HB	2:B:62:LYS:HG2	1.91	0.51
3:C:173:LYS:HA	3:C:178:GLU:HA	1.91	0.51
2:E:86:ARG:NE	2:E:104:SER:O	2.42	0.51
1:G:253:ILE:HG22	1:G:270:LYS:HZ2	1.74	0.51
1:G:415:THR:O	1:G:419:LEU:HD23	2.10	0.51
1:J:226:VAL:HA	1:J:229:LEU:HD23	1.92	0.51
1:J:416:LYS:O	1:J:420:LYS:HG3	2.10	0.51
3:F:149:LEU:HD22	3:F:207:LYS:HZ3	1.76	0.51
1:G:261:LYS:HA	1:G:264:ARG:NH1	2.25	0.51
1:G:304:ARG:NH2	1:G:421:GLU:OE2	2.44	0.51
3:C:169:ASN:OD1	3:C:170:VAL:N	2.44	0.51
3:I:52:ASN:ND2	3:I:54:GLY:C	2.62	0.51
2:B:23:LEU:HD23	2:B:115:CYS:SG	2.50	0.51
3:C:113:GLN:HG2	3:C:114:GLN:N	2.24	0.51
1:G:177:TYR:OH	1:G:380:GLU:OE1	2.24	0.51
1:G:260:PHE:HE2	1:G:270:LYS:HD2	1.76	0.51
1:J:285:LEU:O	1:J:289:ASN:HB2	2.11	0.51
2:H:124:PHE:HE1	3:I:113:GLN:HE22	1.59	0.51
1:D:414:VAL:HG12	1:D:415:THR:H	1.76	0.51
3:F:183:VAL:HB	3:F:203:LEU:HD13	1.92	0.51
2:H:62:LYS:HD2	3:I:111:PHE:HB3	1.93	0.51
3:F:205:LEU:HG	3:F:209:GLU:HG2	1.94	0.50
3:I:47:CYS:HB3	3:I:59:TRP:HE1	1.75	0.50
1:A:187:TYR:OH	1:A:297:LYS:HG2	2.10	0.50
1:A:308:GLU:HA	1:A:416:LYS:HE2	1.93	0.50
2:B:161:THR:HG22	2:B:206:THR:HG22	1.94	0.50
1:D:328:TYR:HB3	1:D:332:PHE:HE1	1.76	0.50
1:G:351:TYR:OH	1:G:378:GLN:O	2.27	0.50
1:J:200:TYR:CE1	1:J:434:LYS:HG3	2.46	0.50
1:A:267:TYR:CE2	1:A:372:ASN:HB3	2.47	0.50
1:A:314:GLN:HA	1:A:415:THR:HA	1.93	0.50
2:B:53:MET:HB3	2:B:98:LEU:HD22	1.93	0.50
3:F:173:LYS:HE2	3:F:219:GLU:HB2	1.93	0.50
2:B:193:VAL:O	2:B:200:THR:N	2.45	0.50
1:D:254:LEU:HD12	1:D:376:PHE:CD2	2.47	0.50
1:D:261:LYS:O	1:D:261:LYS:NZ	2.31	0.50
3:F:145:SER:O	3:F:149:LEU:HG	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:GLU:O	1:A:384:ILE:HG12	2.12	0.50
2:B:32:GLN:HG3	2:B:33:PRO:HD2	1.93	0.50
2:H:80:LEU:O	2:H:84:LYS:N	2.45	0.50
3:I:59:TRP:HZ2	3:I:95:PHE:CB	2.25	0.50
2:B:110:THR:HG22	2:B:135:VAL:N	2.26	0.50
2:B:176:LEU:HD13	2:B:203:SER:HB3	1.94	0.50
3:C:49:ALA:O	3:C:93:THR:HG23	2.12	0.50
3:F:216:TYR:HB2	3:F:231:LYS:HB3	1.93	0.50
3:I:47:CYS:O	3:I:95:PHE:HB2	2.12	0.50
1:D:267:TYR:CZ	1:D:372:ASN:HB3	2.47	0.50
2:B:165:LEU:HD13	2:B:202:SER:HB3	1.93	0.50
1:G:380:GLU:O	1:G:384:ILE:HG13	2.12	0.50
2:H:46:PHE:HB2	2:H:117:ARG:NH1	2.26	0.50
1:D:414:VAL:HG12	1:D:415:THR:N	2.27	0.49
1:G:419:LEU:HD23	1:G:419:LEU:H	1.76	0.49
1:A:279:GLU:O	1:A:283:GLY:N	2.42	0.49
2:B:195:GLN:O	2:B:197:ASP:N	2.46	0.49
3:C:208:ASP:OD1	3:C:209:GLU:HG2	2.12	0.49
1:G:208:TYR:CE2	1:G:426:ILE:HD11	2.47	0.49
3:I:57:VAL:O	3:I:75:ALA:N	2.45	0.49
1:A:299:ILE:O	1:A:303:ILE:HG12	2.11	0.49
3:F:60:TYR:HD1	3:F:70:ALA:HA	1.76	0.49
1:J:222:HIS:HA	1:J:226:VAL:HB	1.93	0.49
1:A:261:LYS:HZ2	1:A:264:ARG:HD2	1.77	0.49
1:A:354:GLY:O	1:A:358:ILE:HG13	2.12	0.49
1:D:263:GLN:OE1	1:D:265:GLU:N	2.35	0.49
2:B:36:SER:O	2:B:36:SER:OG	2.27	0.49
2:E:180:SER:H	2:E:220:ASN:ND2	2.07	0.49
2:H:56:VAL:HG23	2:H:65:GLU:O	2.13	0.49
1:J:326:LYS:HD3	1:J:329:LEU:HD11	1.95	0.49
1:J:358:ILE:HD11	1:J:371:ILE:HG23	1.94	0.49
1:A:196:PHE:HB2	1:A:199:ILE:HD13	1.94	0.49
3:F:210:TYR:HE1	3:F:216:TYR:CE2	2.30	0.49
1:G:453:ILE:O	1:G:457:LEU:HD23	2.13	0.49
1:J:173:ASP:O	1:J:248:LYS:NZ	2.44	0.49
1:J:436:GLY:O	1:J:440:LEU:HG	2.12	0.49
2:E:65:GLU:N	3:F:122:PHE:HZ	2.09	0.48
2:B:55:TRP:CD1	2:B:100:LEU:HD23	2.48	0.48
2:B:171:PRO:O	2:B:223:HIS:NE2	2.46	0.48
1:D:206:LYS:HD3	1:D:222:HIS:CE1	2.48	0.48
2:E:53:MET:HB3	2:E:98:LEU:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:332:PHE:HA	1:J:433:PHE:CZ	2.48	0.48
1:D:446:ALA:O	1:D:450:LYS:HG2	2.13	0.48
1:A:236:ALA:HB1	1:A:288:LYS:HB3	1.94	0.48
3:C:37:THR:O	3:C:130:ILE:HA	2.12	0.48
3:C:132:ARG:HG3	3:C:133:ALA:N	2.29	0.48
2:H:43:ALA:HB3	2:H:48:PHE:CZ	2.48	0.48
1:A:269:VAL:O	1:A:273:GLN:HG3	2.14	0.48
1:A:274:TYR:OH	1:A:380:GLU:OE1	2.21	0.48
3:F:114:GLN:HG2	3:F:116:ASP:H	1.78	0.48
3:F:191:ASP:OD2	3:F:194:ASP:N	2.31	0.48
2:H:47:THR:O	2:H:117:ARG:NH2	2.47	0.48
1:J:303:ILE:HA	1:J:306:LEU:HD22	1.94	0.48
1:A:214:GLU:HG2	1:A:311:LYS:HG3	1.96	0.48
1:G:446:ALA:O	1:G:450:LYS:HG2	2.13	0.48
2:H:39:LEU:HB2	2:H:55:TRP:HZ3	1.78	0.48
1:J:313:SER:HB3	1:J:314:GLN:OE1	2.13	0.48
3:F:34:PHE:CD2	3:F:127:LYS:HB3	2.49	0.48
3:I:86:PHE:HZ	3:I:98:THR:O	1.96	0.48
1:J:181:SER:HA	1:J:188:LEU:HA	1.96	0.48
3:C:205:LEU:HD13	3:C:206:THR:O	2.14	0.48
1:D:448:ILE:O	1:D:452:LYS:HG2	2.14	0.48
2:E:57:ARG:NH2	2:E:109:ASP:OD1	2.47	0.48
2:H:84:LYS:HZ2	2:H:85:SER:H	1.61	0.48
3:I:52:ASN:ND2	3:I:54:GLY:N	2.62	0.47
3:I:78:ARG:NH2	3:I:84:ASP:OD1	2.44	0.47
1:J:394:LYS:HB3	1:J:432:ILE:HD12	1.95	0.47
3:C:61:GLN:HG3	3:C:110:TYR:HE1	1.78	0.47
2:E:69:SER:HB2	2:E:78:TYR:HB2	1.96	0.47
3:F:152:GLY:HA2	3:F:207:LYS:HG3	1.95	0.47
1:A:318:THR:N	1:A:412:LYS:O	2.41	0.47
1:A:381:MET:O	1:A:385:ILE:HG13	2.14	0.47
3:C:190:GLN:NE2	3:C:195:SER:HA	2.30	0.47
3:C:218:CYS:H	3:C:229:ILE:C	2.17	0.47
2:H:50:ASP:OD1	2:H:50:ASP:N	2.46	0.47
3:I:48:LYS:HG2	3:I:49:ALA:O	2.14	0.47
1:A:288:LYS:HD3	1:A:288:LYS:HA	1.71	0.47
1:D:224:THR:HG21	2:E:72:TYR:HD2	1.79	0.47
3:F:114:GLN:OE1	3:F:121:PRO:HD2	2.15	0.47
1:J:219:GLU:HB3	1:J:222:HIS:HB3	1.95	0.47
1:J:374:ILE:HB	1:J:457:LEU:HD22	1.96	0.47
3:C:174:ILE:N	3:C:177:SER:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:170:PHE:N	2:E:223:HIS:HE1	2.11	0.47
2:E:222:ALA:HB2	2:E:229:LYS:HD3	1.96	0.47
1:G:214:GLU:HB2	1:G:310:LEU:HG	1.96	0.47
1:J:192:LEU:HD23	1:J:442:MET:HG2	1.96	0.47
1:J:351:TYR:HD2	1:J:352:LEU:HD22	1.79	0.47
3:I:53:VAL:HG21	3:I:116:ASP:OD2	2.06	0.47
1:A:344:ILE:HD13	1:A:392:LEU:HD23	1.97	0.47
3:F:157:VAL:HG13	3:F:202:THR:HG22	1.97	0.47
3:F:169:ASN:OD1	3:F:170:VAL:N	2.48	0.47
1:G:358:ILE:O	1:G:362:GLU:HB3	2.14	0.47
3:I:59:TRP:CD1	3:I:112:CYS:HB2	2.46	0.47
1:G:397:HIS:CE1	1:G:401:GLN:HG3	2.50	0.47
1:J:175:ILE:HD11	1:J:244:LYS:HG3	1.96	0.47
1:G:386:ASP:O	1:G:390:TYR:N	2.45	0.46
2:H:115:CYS:O	2:H:128:GLY:N	2.48	0.46
1:A:170:ASN:OD1	1:A:170:ASN:N	2.48	0.46
2:B:222:ALA:O	2:B:224:PRO:HD3	2.16	0.46
3:C:59:TRP:CH2	3:C:112:CYS:HB3	2.50	0.46
1:G:240:CYS:O	1:G:244:LYS:N	2.38	0.46
1:G:299:ILE:O	1:G:303:ILE:HG13	2.14	0.46
1:J:419:LEU:HD13	1:J:419:LEU:O	2.15	0.46
2:B:111:ALA:HB3	2:B:113:TYR:CZ	2.50	0.46
1:D:312:CYS:O	1:D:416:LYS:HE2	2.15	0.46
3:F:112:CYS:O	3:F:122:PHE:HB2	2.16	0.46
2:H:127:TRP:CE3	3:I:68:PRO:HG2	2.50	0.46
1:D:182:ASP:HB3	1:D:286:LEU:HD11	1.98	0.46
3:C:179:ARG:NE	3:C:181:ASN:O	2.49	0.46
1:G:251:ILE:HG22	1:G:255:GLU:OE2	2.16	0.46
1:G:247:VAL:HG21	1:G:281:PHE:HB2	1.98	0.46
2:H:61:ASP:HA	2:H:62:LYS:HA	1.56	0.46
3:C:52:ASN:OD1	3:C:92:GLY:HA2	2.16	0.46
3:C:57:VAL:HA	3:C:113:GLN:O	2.15	0.46
1:G:316:CYS:HB2	1:G:419:LEU:HD22	1.97	0.46
2:B:139:LYS:H	2:B:139:LYS:HD3	1.80	0.46
1:D:275:GLU:O	1:D:279:GLU:HG2	2.16	0.46
2:E:171:PRO:CD	2:E:225:ALA:HB3	2.46	0.46
1:J:214:GLU:OE2	1:J:311:LYS:HB3	2.16	0.46
2:B:35:SER:HB2	2:B:103:SER:HA	1.97	0.45
3:C:155:SER:HB3	3:C:204:THR:HG22	1.98	0.45
1:J:207:ARG:HD2	1:J:207:ARG:HA	1.80	0.45
1:J:258:GLN:O	1:J:262:THR:HG23	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:322:PHE:O	1:J:325:ILE:HG22	2.16	0.45
3:F:149:LEU:CD2	3:F:207:LYS:HZ3	2.29	0.45
1:G:256:ASN:HD21	1:G:259:LYS:HB2	1.81	0.45
1:G:393:GLN:O	1:G:393:GLN:NE2	2.48	0.45
1:G:400:ASP:OD1	1:G:401:GLN:N	2.50	0.45
2:B:41:CYS:O	2:B:97:ILE:HA	2.16	0.45
3:C:171:LYS:HE3	3:C:221:THR:OG1	2.16	0.45
2:E:62:LYS:HB2	3:F:111:PHE:CZ	2.52	0.45
3:F:165:PRO:HG3	3:F:223:LYS:HE3	1.99	0.45
1:G:322:PHE:HZ	1:G:411:PRO:HD2	1.81	0.45
2:H:48:PHE:HB3	2:H:91:ARG:NH2	2.31	0.45
1:J:212:HIS:CE1	1:J:216:LYS:HA	2.51	0.45
2:E:212:TRP:CZ2	2:E:236:PRO:HB3	2.52	0.45
3:F:190:GLN:HG3	3:F:197:TYR:CE1	2.52	0.45
1:G:170:ASN:OD1	1:G:171:THR:N	2.50	0.45
2:B:23:LEU:HA	2:B:42:THR:O	2.16	0.45
2:B:204:SER:HB3	3:C:159:PHE:CE2	2.52	0.45
1:G:451:GLU:O	1:G:454:VAL:HG12	2.17	0.45
2:H:55:TRP:HE1	2:H:98:LEU:HD23	1.82	0.45
1:J:197:SER:O	1:J:431:SER:OG	2.35	0.45
1:G:190:SER:HB2	1:G:435:PHE:HZ	1.82	0.45
3:I:45:VAL:O	3:I:97:LEU:HB3	2.16	0.45
1:J:347:TYR:OH	1:J:451:GLU:HB2	2.16	0.45
2:B:73:ASP:OD1	2:B:74:GLY:N	2.50	0.45
2:E:64:LEU:HD23	2:E:64:LEU:HA	1.82	0.45
1:J:258:GLN:HA	1:J:261:LYS:HG3	1.99	0.45
1:J:332:PHE:CD2	1:J:399:ILE:HG22	2.52	0.45
1:A:267:TYR:OH	1:A:376:PHE:HB2	2.16	0.45
1:A:307:LEU:HB2	1:A:420:LYS:HE2	1.98	0.45
1:G:312:CYS:SG	1:G:316:CYS:N	2.90	0.45
1:G:415:THR:O	1:G:418:ARG:N	2.48	0.45
2:H:46:PHE:HB2	2:H:117:ARG:HH12	1.82	0.45
2:E:62:LYS:HA	2:E:63:GLY:C	2.36	0.44
2:E:172:GLU:N	2:E:173:PRO:HD2	2.32	0.44
1:G:220:ASP:OD2	2:H:71:SER:OG	2.34	0.44
2:B:21:VAL:HA	2:B:44:SER:O	2.17	0.44
3:F:154:ALA:O	3:F:205:LEU:N	2.31	0.44
1:G:362:GLU:OE2	1:G:362:GLU:N	2.50	0.44
1:J:225:LYS:O	1:J:229:LEU:N	2.41	0.44
1:J:251:ILE:HG22	1:J:255:GLU:OE1	2.16	0.44
1:J:370:THR:HG23	1:J:371:ILE:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:52:ASN:OD1	3:C:54:GLY:N	2.37	0.44
3:F:44:SER:HA	3:F:97:LEU:O	2.18	0.44
1:A:293:LEU:O	1:A:297:LYS:HG3	2.18	0.44
1:A:328:TYR:O	1:A:332:PHE:N	2.43	0.44
1:D:336:PRO:HD2	1:D:340:TYR:HE1	1.81	0.44
3:F:38:SER:H	3:F:41:VAL:HG22	1.83	0.44
1:G:308:GLU:HA	1:G:416:LYS:HZ3	1.83	0.44
1:G:322:PHE:CZ	1:G:411:PRO:HD2	2.52	0.44
1:J:287:ASN:OD1	1:J:287:ASN:N	2.43	0.44
1:A:388:PHE:CE2	1:A:444:ASN:HB3	2.51	0.44
1:J:297:LYS:HB2	1:J:297:LYS:HE3	1.79	0.44
1:J:394:LYS:HA	1:J:394:LYS:HD2	1.86	0.44
2:B:68:ALA:HB2	2:B:79:TYR:HD1	1.83	0.44
1:D:469:ILE:O	1:D:470:SER:HB3	2.17	0.44
2:E:171:PRO:HB2	2:E:173:PRO:HD2	2.00	0.44
1:G:417:ASN:O	1:G:421:GLU:HG2	2.17	0.44
1:J:363:LYS:H	1:J:363:LYS:HG3	1.67	0.44
1:J:440:LEU:HD12	1:J:441:ASN:N	2.33	0.44
1:A:264:ARG:HA	1:A:264:ARG:NE	2.32	0.44
1:A:266:SER:HB3	1:A:269:VAL:HG22	2.00	0.44
3:I:61:GLN:HG3	3:I:62:GLN:O	2.18	0.44
2:B:59:VAL:O	2:B:62:LYS:HB2	2.18	0.44
3:C:147:GLU:O	3:C:150:THR:OG1	2.33	0.44
1:D:359:ARG:HA	1:D:362:GLU:HG3	2.00	0.44
1:G:331:ASP:OD2	1:G:430:TYR:OH	2.35	0.44
1:J:220:ASP:OD1	1:J:224:THR:OG1	2.36	0.44
2:B:59:VAL:HG12	2:B:60:PRO:HD2	1.99	0.43
3:I:52:ASN:ND2	3:I:54:GLY:CA	2.81	0.43
1:J:178:PHE:CE1	1:J:278:LYS:HE3	2.53	0.43
1:J:307:LEU:HD13	1:J:420:LYS:HG2	1.99	0.43
1:A:244:LYS:HB2	1:A:281:PHE:CE1	2.53	0.43
1:A:390:TYR:HD1	1:A:391:HIS:HD2	1.66	0.43
2:B:113:TYR:O	2:B:130:GLY:HA2	2.18	0.43
2:B:163:GLY:HA2	2:B:204:SER:HA	1.99	0.43
2:B:198:LEU:HD23	2:B:198:LEU:HA	1.79	0.43
3:C:74:SER:O	3:C:76:SER:N	2.45	0.43
2:H:39:LEU:HB2	2:H:55:TRP:CZ3	2.52	0.43
1:J:371:ILE:HD12	1:J:371:ILE:N	2.33	0.43
2:B:22:LYS:C	2:B:23:LEU:HD12	2.38	0.43
2:B:55:TRP:CE3	2:B:113:TYR:HB3	2.54	0.43
2:B:111:ALA:HB3	2:B:113:TYR:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:173:PRO:O	2:B:224:PRO:HD2	2.18	0.43
2:E:62:LYS:H	2:E:62:LYS:HD2	1.83	0.43
3:F:59:TRP:HB2	3:F:72:ILE:HB	1.98	0.43
1:G:310:LEU:HD22	1:G:311:LYS:HG2	2.01	0.43
3:I:61:GLN:HG3	3:I:62:GLN:N	2.33	0.43
1:A:365:ILE:H	1:A:365:ILE:HG13	1.67	0.43
2:B:141:THR:N	2:B:170:PHE:O	2.45	0.43
1:D:354:GLY:O	1:D:358:ILE:HG13	2.18	0.43
3:F:147:GLU:O	3:F:150:THR:HG22	2.18	0.43
3:C:48:LYS:O	3:C:49:ALA:HB2	2.17	0.43
1:D:347:TYR:CE2	1:D:447:LEU:HD22	2.54	0.43
1:G:344:ILE:HD12	1:G:344:ILE:HA	1.89	0.43
1:G:364:GLN:N	1:G:364:GLN:OE1	2.52	0.43
3:I:48:LYS:HG2	3:I:49:ALA:N	2.33	0.43
1:A:387:ARG:HA	1:A:387:ARG:HD3	1.68	0.43
1:D:206:LYS:HD3	1:D:222:HIS:ND1	2.33	0.43
1:D:374:ILE:O	1:D:378:GLN:HG3	2.18	0.43
2:E:188:HIS:NE2	3:F:188:THR:HG21	2.34	0.43
2:E:212:TRP:CH2	2:E:236:PRO:HB3	2.54	0.43
1:G:172:THR:HG22	1:G:449:HIS:CE1	2.53	0.43
1:G:247:VAL:O	1:G:251:ILE:HG13	2.19	0.43
1:J:410:LYS:N	1:J:411:PRO:CD	2.82	0.43
2:B:24:VAL:O	2:B:41:CYS:HA	2.19	0.43
1:D:419:LEU:HA	1:D:422:TYR:HB2	2.01	0.43
1:G:325:ILE:HG22	1:G:426:ILE:HG21	2.00	0.43
3:C:39:ILE:HA	3:C:40:GLY:HA2	1.54	0.43
3:C:179:ARG:HD3	3:C:203:LEU:HD11	1.99	0.43
1:D:441:ASN:O	1:D:445:LYS:HG3	2.19	0.43
1:G:422:TYR:HA	1:G:425:ASN:ND2	2.34	0.43
2:H:54:ALA:O	2:H:116:THR:OG1	2.21	0.43
3:C:175:ASP:HA	3:C:213:HIS:ND1	2.34	0.43
1:D:176:ASP:HB2	1:D:191:GLN:HG2	2.00	0.43
1:G:273:GLN:O	1:G:277:LYS:HG2	2.19	0.43
1:J:336:PRO:HB2	1:J:339:ASN:HB2	2.01	0.43
2:E:86:ARG:HG2	2:E:104:SER:HB2	2.00	0.43
1:G:266:SER:HB3	1:G:269:VAL:HG22	2.00	0.43
1:A:310:LEU:O	1:A:416:LYS:NZ	2.34	0.42
2:B:38:ASN:OD1	2:B:101:GLN:HA	2.19	0.42
1:G:260:PHE:CE2	1:G:270:LYS:HD2	2.53	0.42
1:G:328:TYR:HE2	1:G:426:ILE:HD13	1.84	0.42
1:J:279:GLU:O	1:J:283:GLY:N	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:446:ALA:O	1:J:450:LYS:HG2	2.19	0.42
2:B:59:VAL:H	2:B:62:LYS:CG	2.32	0.42
2:E:174:VAL:HG13	2:E:222:ALA:O	2.18	0.42
1:A:275:GLU:O	1:A:279:GLU:HG2	2.19	0.42
2:B:58:GLN:N	2:B:112:THR:O	2.52	0.42
1:D:222:HIS:HA	1:D:226:VAL:CG1	2.48	0.42
3:F:134:ASP:OD2	3:F:223:LYS:NZ	2.36	0.42
1:G:312:CYS:SG	1:G:315:ASP:C	2.98	0.42
1:G:373:ALA:O	1:G:377:THR:HG23	2.18	0.42
2:H:40:SER:HA	2:H:98:LEU:O	2.18	0.42
2:H:55:TRP:CD1	2:H:115:CYS:HA	2.54	0.42
1:D:227:ASN:OD1	1:D:228:SER:N	2.52	0.42
1:G:260:PHE:HE1	1:G:264:ARG:HA	1.83	0.42
1:A:316:CYS:HB3	1:A:419:LEU:HD22	2.01	0.42
1:A:374:ILE:CG1	1:A:457:LEU:HD22	2.49	0.42
1:D:336:PRO:HD2	1:D:340:TYR:CE1	2.54	0.42
2:E:210:SER:O	2:E:213:PRO:HD2	2.19	0.42
1:J:242:ARG:O	1:J:246:THR:HG23	2.19	0.42
1:J:275:GLU:O	1:J:279:GLU:HG2	2.19	0.42
2:B:62:LYS:HA	2:B:62:LYS:HD3	1.68	0.42
1:D:183:GLU:OE1	1:D:183:GLU:N	2.46	0.42
1:D:254:LEU:HD12	1:D:376:PHE:CG	2.55	0.42
2:H:57:ARG:HB3	2:H:113:TYR:CD1	2.54	0.42
3:I:62:GLN:HB3	3:I:68:PRO:HA	2.01	0.42
1:J:405:LEU:O	1:J:409:VAL:HG22	2.19	0.42
1:A:368:PRO:HB2	1:A:372:ASN:OD1	2.20	0.42
2:B:59:VAL:CG1	2:B:60:PRO:HD2	2.49	0.42
3:C:190:GLN:HE21	3:C:195:SER:HA	1.84	0.42
3:F:57:VAL:HA	3:F:113:GLN:O	2.20	0.42
1:J:332:PHE:CE2	1:J:402:VAL:HG21	2.51	0.42
1:J:374:ILE:CA	1:J:457:LEU:HD13	2.50	0.42
1:A:451:GLU:O	1:A:454:VAL:HG12	2.20	0.42
2:B:27:GLU:HA	2:B:28:GLY:HA3	1.76	0.42
2:B:180:SER:H	2:B:220:ASN:ND2	2.18	0.42
1:G:232:GLU:CG	1:G:292:ASN:HD21	2.33	0.42
2:H:83:LEU:HD12	2:H:87:PHE:CZ	2.55	0.42
2:H:98:LEU:HD12	2:H:99:ASN:H	1.83	0.42
1:J:460:GLU:O	1:J:464:HIS:N	2.52	0.42
3:C:28:MET:HB2	3:C:50:SER:N	2.16	0.42
2:E:66:TRP:HZ3	3:F:118:TYR:CE2	2.38	0.42
1:J:192:LEU:CD2	1:J:442:MET:HG2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:340:TYR:CZ	1:J:440:LEU:HD13	2.55	0.42
1:A:340:TYR:HD1	1:A:388:PHE:HZ	1.67	0.42
1:A:393:GLN:O	1:A:397:HIS:N	2.47	0.42
2:E:109:ASP:C	2:E:111:ALA:H	2.24	0.42
1:G:214:GLU:OE2	1:G:309:LYS:HE3	2.20	0.42
1:G:449:HIS:O	1:G:453:ILE:HG22	2.20	0.42
3:C:113:GLN:HE21	3:C:120:TYR:HB3	1.85	0.41
1:G:468:ARG:NE	1:G:468:ARG:HA	2.34	0.41
2:H:83:LEU:HD12	2:H:87:PHE:CE2	2.54	0.41
1:J:289:ASN:OD1	1:J:292:ASN:ND2	2.47	0.41
1:D:309:LYS:NZ	2:E:122:ASP:OD2	2.44	0.41
1:G:260:PHE:O	1:G:264:ARG:HG2	2.20	0.41
1:J:286:LEU:O	1:J:290:ARG:HB2	2.20	0.41
1:J:318:THR:OG1	1:J:412:LYS:HA	2.21	0.41
2:B:118:VAL:HG22	2:B:124:PHE:CD1	2.56	0.41
1:D:244:LYS:HB2	1:D:281:PHE:CE1	2.55	0.41
3:F:148:GLN:OE1	3:F:155:SER:OG	2.28	0.41
1:G:232:GLU:HG2	1:G:292:ASN:HD21	1.84	0.41
3:I:53:VAL:HG23	3:I:54:GLY:N	2.35	0.41
2:B:227:SER:O	2:B:227:SER:OG	2.29	0.41
3:C:42:ARG:HA	3:C:99:ILE:O	2.20	0.41
1:D:243:ALA:O	1:D:247:VAL:HG23	2.21	0.41
1:D:264:ARG:HD2	1:D:265:GLU:N	2.35	0.41
1:G:253:ILE:HG22	1:G:270:LYS:NZ	2.35	0.41
1:J:419:LEU:HD22	1:J:422:TYR:HB2	2.02	0.41
2:E:148:LEU:HD11	3:F:142:PHE:HB3	2.03	0.41
3:F:164:TYR:CD1	3:F:165:PRO:HA	2.55	0.41
1:G:397:HIS:O	1:G:397:HIS:ND1	2.54	0.41
2:H:90:SER:N	2:H:99:ASN:O	2.30	0.41
1:A:338:GLU:OE1	1:A:338:GLU:N	2.31	0.41
2:E:169:TYR:OH	2:E:201:LEU:HD23	2.19	0.41
2:E:223:HIS:HB3	2:E:226:SER:HB2	2.02	0.41
2:B:180:SER:H	2:B:220:ASN:HD21	1.69	0.41
1:D:340:TYR:HD2	1:D:388:PHE:CZ	2.37	0.41
1:D:394:LYS:HA	1:D:394:LYS:HD3	1.77	0.41
2:E:149:ALA:O	3:F:143:PRO:HD2	2.21	0.41
1:G:337:TYR:CE2	1:G:396:LYS:HD3	2.56	0.41
1:G:366:ASP:HB3	1:G:468:ARG:CD	2.50	0.41
3:I:55:THR:HA	3:I:95:PHE:CE1	2.55	0.41
3:I:56:ASN:C	3:I:74:SER:HA	2.41	0.41
3:I:112:CYS:SG	3:I:112:CYS:O	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:LEU:HA	1:A:332:PHE:HB2	2.03	0.41
2:B:35:SER:OG	2:B:36:SER:N	2.53	0.41
1:D:295:GLN:O	1:D:299:ILE:HG13	2.20	0.41
2:E:119:THR:HG1	2:E:123:SER:N	2.19	0.41
1:G:340:TYR:CE1	1:G:440:LEU:HB3	2.55	0.41
2:H:79:TYR:CE1	2:H:89:ILE:HG22	2.56	0.41
1:A:399:ILE:O	1:A:403:THR:OG1	2.19	0.41
1:A:441:ASN:O	1:A:444:ASN:ND2	2.54	0.41
2:B:139:LYS:HD3	2:B:139:LYS:N	2.36	0.41
2:B:179:ASN:CA	2:B:217:ILE:HG21	2.40	0.41
2:B:218:THR:HG23	2:B:232:LYS:O	2.21	0.41
2:E:35:SER:HB3	2:E:105:LEU:HD11	2.03	0.41
2:E:58:GLN:NE2	2:E:62:LYS:HE3	2.36	0.41
2:E:143:PRO:HD3	2:E:223:HIS:ND1	2.36	0.41
3:F:219:GLU:HG3	3:F:228:PRO:HB3	2.01	0.41
1:G:197:SER:HB2	1:G:435:PHE:CD2	2.56	0.41
1:G:298:LYS:O	1:G:302:GLU:HG3	2.20	0.41
1:G:368:PRO:HA	1:G:371:ILE:HG12	2.02	0.41
1:G:386:ASP:OD1	1:G:386:ASP:N	2.45	0.41
1:G:394:LYS:HA	1:G:394:LYS:HD3	1.93	0.41
1:J:225:LYS:C	1:J:229:LEU:HD23	2.40	0.41
1:J:438:ASP:N	1:J:438:ASP:OD1	2.54	0.41
1:D:217:ARG:HH21	1:D:221:ILE:HD11	1.86	0.41
1:D:347:TYR:OH	1:D:451:GLU:HB2	2.21	0.41
3:F:54:GLY:H	3:F:92:GLY:HA2	1.86	0.41
1:J:217:ARG:HE	1:J:306:LEU:HG	1.83	0.41
1:J:254:LEU:HB3	1:J:376:PHE:CE2	2.56	0.41
1:J:427:GLY:O	1:J:430:TYR:N	2.54	0.41
1:A:441:ASN:HA	1:A:444:ASN:HD21	1.86	0.40
3:C:55:THR:O	3:C:74:SER:HA	2.21	0.40
1:D:180:ILE:HD12	1:D:282:ARG:HB3	2.03	0.40
1:D:253:ILE:HG23	1:D:260:PHE:HA	2.02	0.40
1:G:306:LEU:HG	2:H:120:VAL:HG12	2.02	0.40
1:G:385:ILE:O	1:G:389:GLU:N	2.40	0.40
1:G:410:LYS:HA	1:G:410:LYS:HD2	1.91	0.40
1:J:366:ASP:OD1	1:J:367:ASN:N	2.54	0.40
2:B:174:VAL:HG13	2:B:222:ALA:O	2.21	0.40
1:D:215:ILE:HG13	1:D:306:LEU:HG	2.03	0.40
1:G:359:ARG:CD	1:J:290:ARG:HE	2.35	0.40
1:J:254:LEU:HD11	1:J:270:LYS:CB	2.50	0.40
1:J:299:ILE:O	1:J:303:ILE:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:385:ILE:O	1:D:389:GLU:HG3	2.21	0.40
1:A:447:LEU:HD23	1:A:447:LEU:HA	1.83	0.40
1:G:269:VAL:O	1:G:273:GLN:HG2	2.21	0.40
3:I:55:THR:HA	3:I:95:PHE:HE1	1.85	0.40
1:A:267:TYR:OH	1:A:372:ASN:O	2.36	0.40
1:A:454:VAL:O	1:A:458:LEU:HG	2.22	0.40
2:B:98:LEU:HD23	2:B:115:CYS:SG	2.61	0.40
2:B:149:ALA:O	3:C:143:PRO:HD2	2.22	0.40
3:C:61:GLN:CB	3:C:71:LEU:HD11	2.51	0.40
2:H:81:ASP:HA	2:H:84:LYS:HB2	2.03	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	297/307 (97%)	289 (97%)	8 (3%)	0	100	100
1	D	300/307 (98%)	295 (98%)	4 (1%)	1 (0%)	41	72
1	G	300/307 (98%)	289 (96%)	11 (4%)	0	100	100
1	J	295/307 (96%)	284 (96%)	10 (3%)	1 (0%)	41	72
2	B	205/254 (81%)	193 (94%)	10 (5%)	2 (1%)	15	49
2	E	204/254 (80%)	192 (94%)	10 (5%)	2 (1%)	15	49
2	H	111/254 (44%)	107 (96%)	4 (4%)	0	100	100
3	C	195/238 (82%)	183 (94%)	10 (5%)	2 (1%)	15	49
3	F	192/238 (81%)	180 (94%)	12 (6%)	0	100	100
3	I	61/238 (26%)	56 (92%)	5 (8%)	0	100	100
All	All	2160/2704 (80%)	2068 (96%)	84 (4%)	8 (0%)	34	68

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	179	ASN
3	C	52	ASN
3	C	228	PRO
1	D	336	PRO
2	E	224	PRO
2	B	64	LEU
2	B	196	SER
1	J	410	LYS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	281/286 (98%)	270 (96%)	11 (4%)	32 63
1	D	284/286 (99%)	277 (98%)	7 (2%)	47 74
1	G	284/286 (99%)	261 (92%)	23 (8%)	11 39
1	J	279/286 (98%)	260 (93%)	19 (7%)	16 47
2	B	187/227 (82%)	177 (95%)	10 (5%)	22 56
2	E	186/227 (82%)	176 (95%)	10 (5%)	22 55
2	H	101/227 (44%)	94 (93%)	7 (7%)	15 47
3	C	175/211 (83%)	173 (99%)	2 (1%)	73 86
3	F	175/211 (83%)	164 (94%)	11 (6%)	18 49
3	I	58/211 (28%)	51 (88%)	7 (12%)	5 21
All	All	2010/2458 (82%)	1903 (95%)	107 (5%)	22 56

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	200	TYR
1	A	217	ARG
1	A	242	ARG
1	A	258	GLN

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Mol	Chain	Res	Type
1	A	272	ARG
1	A	312	CYS
1	A	314	GLN
1	A	357	MET
1	A	362	GLU
1	A	410	LYS
1	A	421	GLU
2	B	20	GLU
2	B	37	MET
2	B	52	TYR
2	B	64	LEU
2	B	122	ASP
2	B	139	LYS
2	B	169	TYR
2	B	179	ASN
2	B	219	CYS
2	B	233	LYS
3	C	94	GLU
3	C	114	GLN
1	D	182	ASP
1	D	217	ARG
1	D	241	ASN
1	D	264	ARG
1	D	364	GLN
1	D	418	ARG
1	D	458	LEU
2	E	38	ASN
2	E	46	PHE
2	E	52	TYR
2	E	58	GLN
2	E	61	ASP
2	E	96	ASN
2	E	139	LYS
2	E	164	CYS
2	E	229	LYS
2	E	232	LYS
3	F	33	LYS
3	F	47	CYS
3	F	79	ASN
3	F	114	GLN
3	F	122	PHE
3	F	132	ARG

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Mol	Chain	Res	Type
3	F	148	GLN
3	F	166	LYS
3	F	178	GLU
3	F	199	MET
3	F	207	LYS
1	G	177	TYR
1	G	187	TYR
1	G	198	ASN
1	G	208	TYR
1	G	217	ARG
1	G	260	PHE
1	G	261	LYS
1	G	285	LEU
1	G	308	GLU
1	G	310	LEU
1	G	311	LYS
1	G	312	CYS
1	G	315	ASP
1	G	348	LYS
1	G	357	MET
1	G	392	LEU
1	G	419	LEU
1	G	434	LYS
1	G	438	ASP
1	G	442	MET
1	G	457	LEU
1	G	462	PHE
1	G	468	ARG
2	H	37	MET
2	H	41	CYS
2	H	52	TYR
2	H	61	ASP
2	H	72	TYR
2	H	115	CYS
2	H	129	GLN
3	I	51	GLN
3	I	60	TYR
3	I	69	LYS
3	I	86	PHE
3	I	111	PHE
3	I	112	CYS
3	I	118	TYR

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Mol	Chain	Res	Type
1	J	183	GLU
1	J	186	TYR
1	J	201	PHE
1	J	207	ARG
1	J	211	TYR
1	J	212	HIS
1	J	217	ARG
1	J	229	LEU
1	J	260	PHE
1	J	293	LEU
1	J	294	ASP
1	J	322	PHE
1	J	331	ASP
1	J	363	LYS
1	J	366	ASP
1	J	372	ASN
1	J	387	ARG
1	J	423	TYR
1	J	435	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	444	ASN
3	C	32	GLN
2	E	38	ASN
2	E	58	GLN
2	E	179	ASN
3	F	62	GLN
3	F	190	GLN
1	G	292	ASN
1	G	372	ASN
3	I	113	GLN
1	J	455	HIS

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 monosaccharides 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, 95^{th} 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	299/307 (97%)	0.24	10 (3%) 46 45	28, 67, 115, 149	0
1	D	302/307 (98%)	0.28	14 (4%) 32 33	36, 72, 116, 173	0
1	G	302/307 (98%)	0.30	7 (2%) 60 60	41, 85, 140, 181	0
1	J	297/307 (96%)	0.35	11 (3%) 41 40	69, 109, 149, 189	0
2	B	209/254 (82%)	0.52	17 (8%) 12 12	31, 72, 135, 165	0
2	E	208/254 (81%)	0.42	17 (8%) 11 12	34, 86, 130, 144	0
2	H	113/254 (44%)	0.70	14 (12%) 4 3	56, 86, 153, 180	0
3	C	199/238 (83%)	0.44	14 (7%) 16 17	34, 79, 130, 176	0
3	F	198/238 (83%)	0.38	8 (4%) 38 37	38, 74, 130, 170	0
3	I	67/238 (28%)	0.83	9 (13%) 3 3	81, 117, 163, 192	0
All	All	2194/2704 (81%)	0.38	121 (5%) 25 26	28, 82, 140, 192	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	64	LEU	6.8
3	I	60	TYR	6.5
1	J	213	THR	6.3
1	J	211	TYR	6.1
2	B	62	LYS	5.5
1	D	464	HIS	4.9
2	E	164	CYS	4.7
2	B	95	LYS	4.7
2	H	78	TYR	4.6
3	C	154	ALA	4.5
2	H	67	VAL	4.5
2	B	161	THR	4.4
2	H	52	TYR	4.3

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Mol	Chain	Res	Type	RSRZ
3	C	28	MET	4.3
2	H	36	SER	4.2
2	E	214	SER	4.2
3	I	71	LEU	4.1
1	J	210	SER	4.0
1	A	215	ILE	3.9
3	C	100	SER	3.9
2	B	162	LEU	3.7
2	E	176	LEU	3.5
2	B	146	TYR	3.5
3	I	59	TRP	3.5
3	I	87	THR	3.4
2	H	48	PHE	3.4
3	F	37	THR	3.4
2	E	187	VAL	3.3
1	D	205	PHE	3.3
1	D	371	ILE	3.3
3	C	223	LYS	3.3
1	G	187	TYR	3.3
3	I	111	PHE	3.2
2	B	65	GLU	3.2
2	H	70	VAL	3.1
3	C	149	LEU	3.1
2	H	68	ALA	3.1
3	C	133	ALA	3.1
3	C	143	PRO	3.0
2	B	19	CYS	3.0
1	D	389	GLU	3.0
2	E	56	VAL	3.0
1	G	215	ILE	3.0
1	J	217	ARG	3.0
1	J	229	LEU	3.0
2	B	94	VAL	3.0
3	F	128	LEU	2.9
1	A	313	SER	2.9
2	E	165	LEU	2.9
3	C	115	TYR	2.9
1	A	457	LEU	2.9
1	G	309	LYS	2.9
2	H	118	VAL	2.8
1	G	208	TYR	2.8
1	G	413	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	453	ILE	2.8
1	G	285	LEU	2.8
2	H	72	TYR	2.8
2	H	79	TYR	2.8
2	E	162	LEU	2.7
2	E	178	TRP	2.7
1	J	432	ILE	2.7
3	F	108	ALA	2.7
1	D	271	LEU	2.7
2	B	63	GLY	2.7
1	D	285	LEU	2.6
1	J	187	TYR	2.6
1	D	226	VAL	2.6
2	B	136	SER	2.5
2	H	119	THR	2.5
1	J	426	ILE	2.5
2	E	55	TRP	2.5
2	H	53	MET	2.5
2	E	161	THR	2.5
2	E	146	TYR	2.4
1	D	307	LEU	2.4
3	C	83	PRO	2.4
1	A	464	HIS	2.4
3	F	131	LYS	2.4
1	J	207	ARG	2.4
3	F	39	ILE	2.4
1	A	324	MET	2.4
1	A	173	ASP	2.3
1	G	408	GLY	2.3
2	B	206	THR	2.3
3	C	113	GLN	2.3
3	C	186	SER	2.3
3	I	116	ASP	2.3
1	D	306	LEU	2.3
1	A	211	TYR	2.3
2	B	160	VAL	2.3
1	J	283	GLY	2.2
3	C	123	GLY	2.2
2	B	150	PRO	2.2
2	H	89	ILE	2.2
2	E	62	LYS	2.2
2	E	145	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
3	I	115	TYR	2.2
3	F	220	ALA	2.2
2	E	125	ASP	2.1
2	B	216	SER	2.1
1	A	307	LEU	2.1
1	D	347	TYR	2.1
2	B	207	VAL	2.1
1	D	251	ILE	2.1
2	B	214	SER	2.1
3	C	155	SER	2.1
3	C	32	GLN	2.1
3	I	61	GLN	2.1
2	E	236	PRO	2.1
1	D	274	TYR	2.1
2	E	199	TYR	2.1
3	F	29	THR	2.1
3	F	216	TYR	2.1
3	I	57	VAL	2.1
1	J	423	TYR	2.0
1	A	322	PHE	2.0
2	E	205	VAL	2.0
1	D	303	ILE	2.0
1	D	318	THR	2.0
2	H	123	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no 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.