Full wwPDB X-ray Structure Validation Report (i)

Dec 18, 2024 – 04:11 PM EST

PDB ID	:	8SJA
Title	:	Ara H 6 13D9 16A8
Authors	:	Spiller, B.W.; Shrem, R.A.
Deposited on	:	2023-04-17
Resolution	:	2.68 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 (i) 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 (1)) were used in the production of this report:

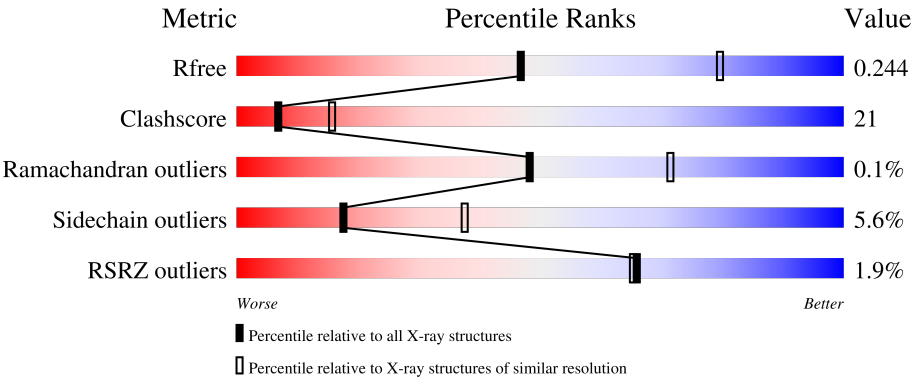
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.68 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	4708 (2.70-2.66)
Clashscore	180529	5138 (2.70-2.66)
Ramachandran outliers	177936	5071 (2.70-2.66)
Sidechain outliers	177891	5071 (2.70-2.66)
RSRZ outliers	164620	4708 (2.70-2.66)

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	215	4% 61% 34%
1	L	215	% 67% 29%
2	B	224	3% 67% 27%
2	H	224	% 65% 28% 5%
3	G	122	47% 29% 21%

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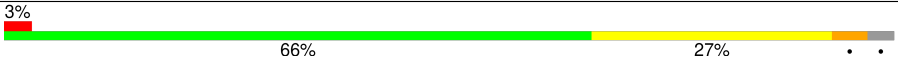
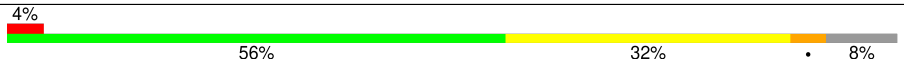
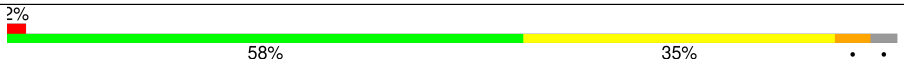
Mol	Chain	Length	Quality of chain
3	I	122	
4	C	212	
4	E	212	
5	D	224	
5	F	224	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	ACT	L	301	-	X	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14530 atoms, of which 6 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 16A8 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	210	Total	C	N	O	S	0	0	0
			1603	998	276	324	5			
1	A	210	Total	C	N	O	S	0	0	0
			1603	998	276	324	5			

- Molecule 2 is a protein called 16A8 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	219	Total	C	N	O	S	0	0	0
			1651	1042	272	331	6			
2	B	214	Total	C	N	O	S	0	0	0
			1616	1023	266	321	6			

- Molecule 3 is a protein called Conglutin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	96	Total	C	N	O	S	0	0	0
			786	461	152	156	17			
3	I	95	Total	C	N	O	S	0	0	0
			779	457	151	154	17			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	12	MET	-	initiating methionine	UNP Q647G9
G	70	GLY	ARG	conflict	UNP Q647G9
G	102	SER	ASN	conflict	UNP Q647G9
G	125	SER	-	expression tag	UNP Q647G9
G	126	GLY	-	expression tag	UNP Q647G9
G	127	SER	-	expression tag	UNP Q647G9
G	128	HIS	-	expression tag	UNP Q647G9
G	129	HIS	-	expression tag	UNP Q647G9

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Chain	Residue	Modelled	Actual	Comment	Reference
G	130	HIS	-	expression tag	UNP Q647G9
G	131	HIS	-	expression tag	UNP Q647G9
G	132	HIS	-	expression tag	UNP Q647G9
G	133	HIS	-	expression tag	UNP Q647G9
I	12	MET	-	initiating methionine	UNP Q647G9
I	70	GLY	ARG	conflict	UNP Q647G9
I	102	SER	ASN	conflict	UNP Q647G9
I	125	SER	-	expression tag	UNP Q647G9
I	126	GLY	-	expression tag	UNP Q647G9
I	127	SER	-	expression tag	UNP Q647G9
I	128	HIS	-	expression tag	UNP Q647G9
I	129	HIS	-	expression tag	UNP Q647G9
I	130	HIS	-	expression tag	UNP Q647G9
I	131	HIS	-	expression tag	UNP Q647G9
I	132	HIS	-	expression tag	UNP Q647G9
I	133	HIS	-	expression tag	UNP Q647G9

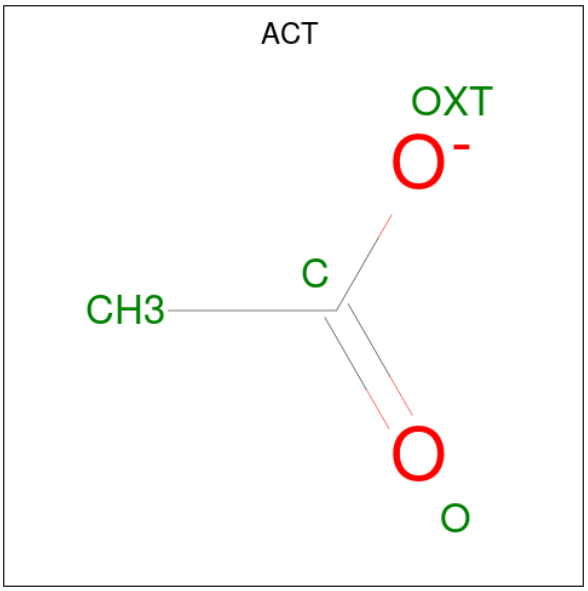
- Molecule 4 is a protein called 13D9 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	206	Total	C	N	O	S	0	0	0
			1556	972	260	320	4			
4	E	212	Total	C	N	O	S	0	0	0
			1596	995	266	330	5			

- Molecule 5 is a protein called 13D9 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	206	Total	C	N	O	S	0	0	0
			1551	984	263	296	8			
5	F	217	Total	C	N	O	S	0	0	0
			1626	1030	275	313	8			

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	L	1	Total C H O 7 2 3 2	0	0
6	A	1	Total C H O 7 2 3 2	0	0

- Molecule 7 is water.

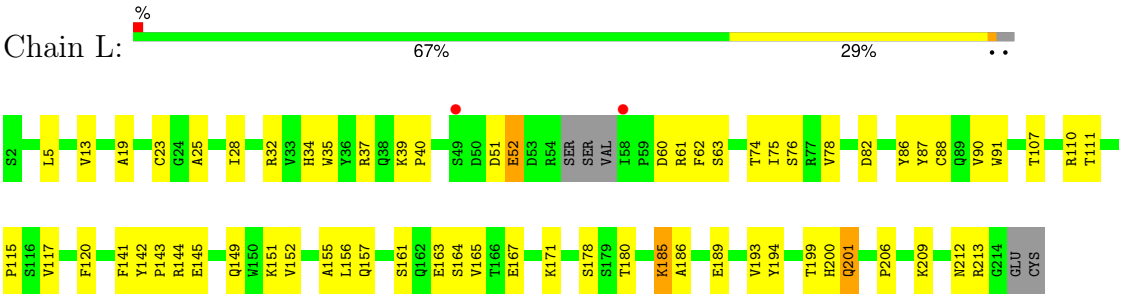
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	15	Total O 15 15	0	0
7	H	37	Total O 37 37	0	0
7	B	17	Total O 17 17	0	0
7	G	2	Total O 2 2	0	0
7	I	3	Total O 3 3	0	0
7	C	14	Total O 14 14	0	0
7	D	6	Total O 6 6	0	0
7	E	34	Total O 34 34	0	0
7	F	9	Total O 9 9	0	0
7	A	12	Total O 12 12	0	0

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.

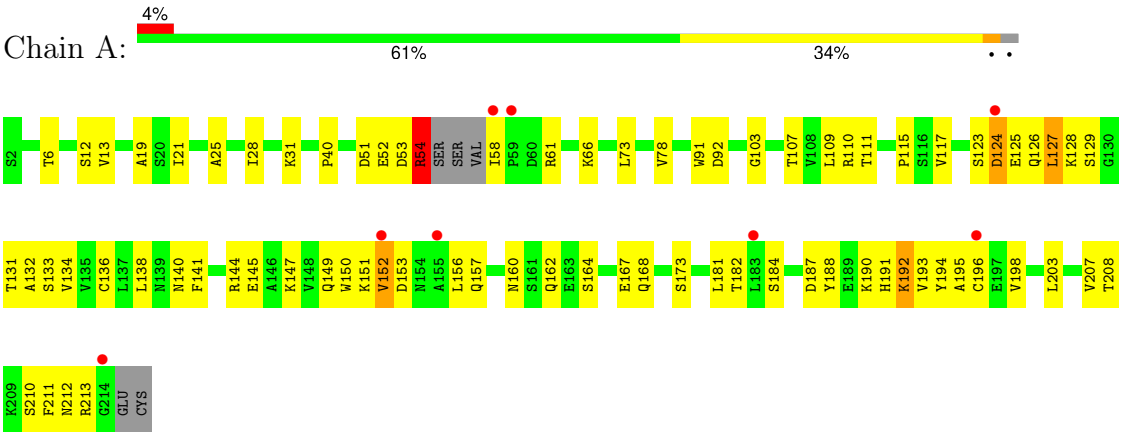
• Molecule 1: 16A8 light chain

Chain L:



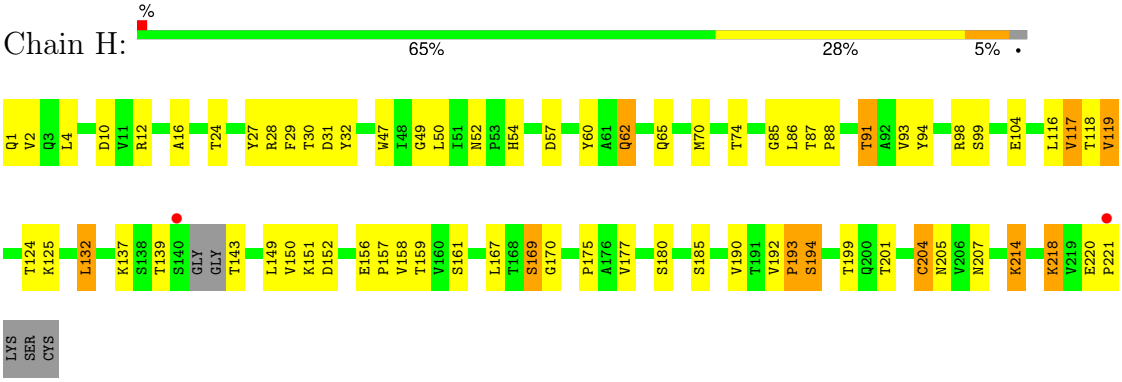
• Molecule 1: 16A8 light chain

Chain A:



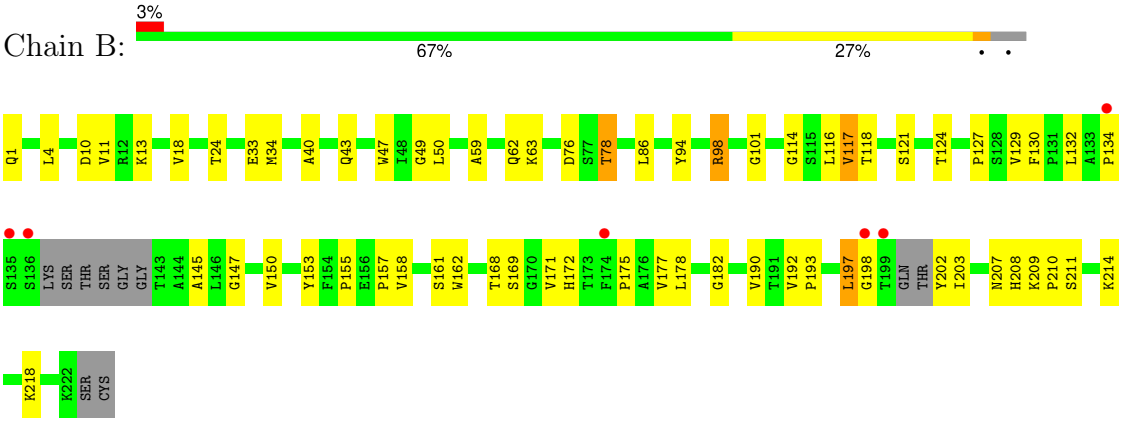
• Molecule 2: 16A8 heavy chain

Chain H:



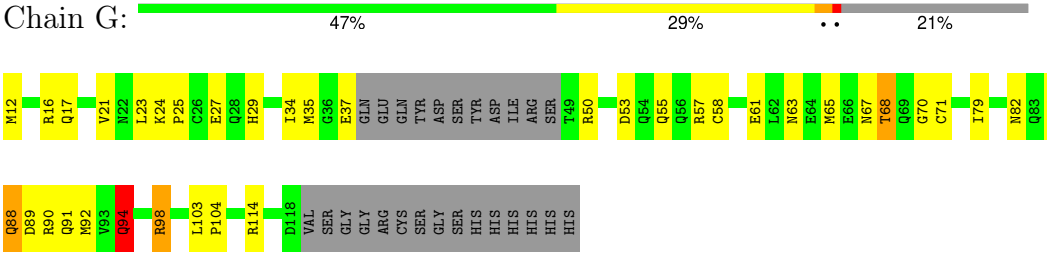
• Molecule 2: 16A8 heavy chain

Chain B:



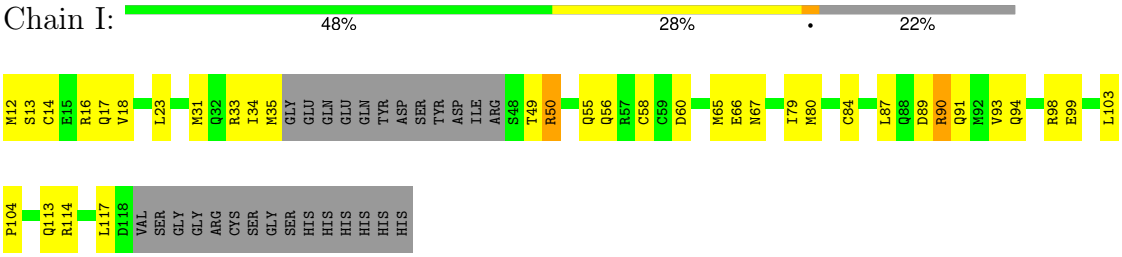
• Molecule 3: Conglutin

Chain G:



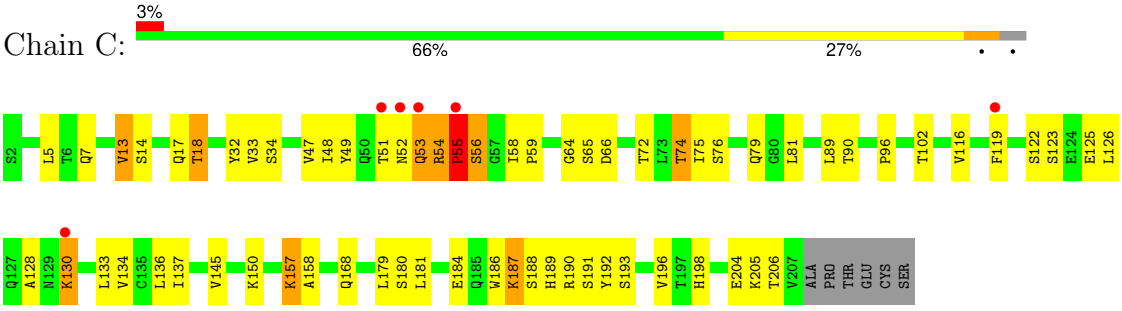
• Molecule 3: Conglutin

Chain I:



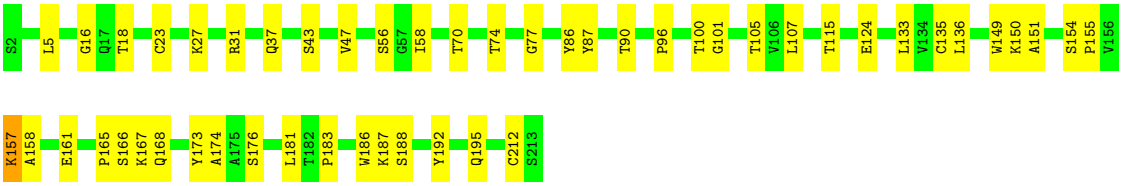
• Molecule 4: 13D9 light chain

Chain C:

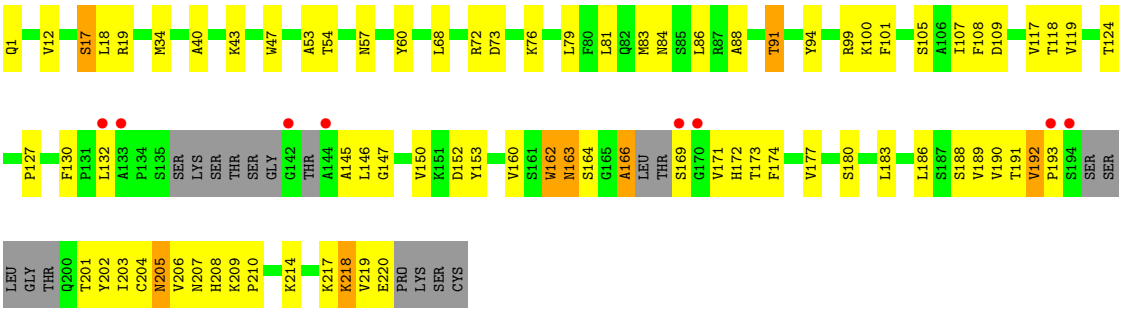


• Molecule 4: 13D9 light chain

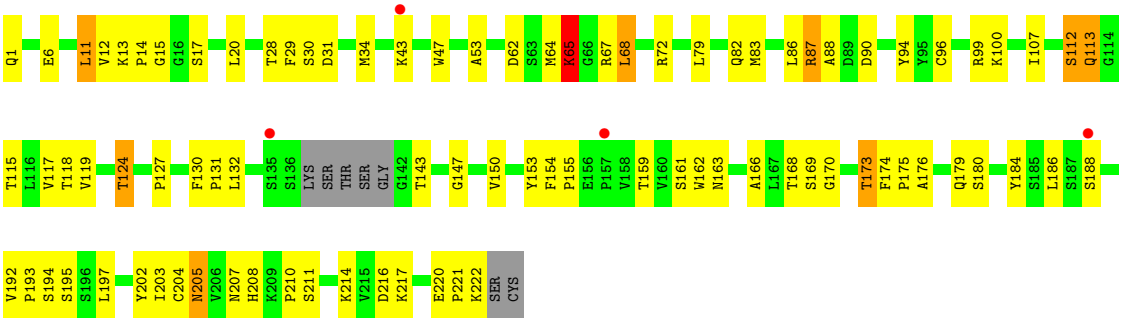
Chain E:



• Molecule 5: 13D9 heavy chain



• Molecule 5: 13D9 heavy chain



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	108.47Å 112.07Å 223.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.96 – 2.68 44.96 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.3 (44.96-2.68) 99.3 (44.96-2.69)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.194 , 0.239 0.196 , 0.244	Depositor DCC
R_{free} test set	3936 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å^2)	68.2	Xtriage
Anisotropy	0.367	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 59.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14530	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

Bond lengths and bond angles in the following residue types are not validated in this section: ACT

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	0.49	0/1637	0.77	6/2226 (0.3%)
1	L	0.52	0/1637	0.80	4/2226 (0.2%)
2	B	0.51	0/1656	0.70	0/2261
2	H	0.60	0/1692	0.74	2/2312 (0.1%)
3	G	0.56	0/790	0.91	3/1051 (0.3%)
3	I	0.60	0/783	0.75	0/1042
4	C	0.52	1/1594 (0.1%)	0.73	1/2178 (0.0%)
4	E	0.53	0/1635	0.69	0/2235
5	D	0.59	2/1585 (0.1%)	0.73	1/2146 (0.0%)
5	F	0.55	0/1664	0.91	7/2259 (0.3%)
All	All	0.55	3/14673 (0.0%)	0.77	24/19936 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	H	0	2
3	G	0	1
5	F	0	2
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	166	ALA	CA-CB	7.09	1.67	1.52
5	D	162	TRP	CB-CG	6.39	1.61	1.50
4	C	130	LYS	CD-CE	-5.56	1.37	1.51

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	65	LYS	CB-CG-CD	-13.94	75.35	111.60
5	F	113	GLN	CA-CB-CG	-13.08	84.63	113.40
5	F	65	LYS	CB-CA-C	-12.11	86.19	110.40
3	G	94	GLN	CA-CB-CG	11.72	139.19	113.40
5	F	65	LYS	CA-CB-CG	10.26	135.97	113.40
1	L	52	GLU	CG-CD-OE2	-8.99	100.32	118.30
1	A	127	LEU	CB-CG-CD2	-8.82	96.00	111.00
1	L	51	ASP	C-N-CA	8.55	143.08	121.70
1	A	192	LYS	CA-CB-CG	8.10	131.21	113.40
3	G	94	GLN	CB-CA-C	-7.38	95.64	110.40
1	L	52	GLU	N-CA-CB	-7.22	97.59	110.60
5	F	112	SER	C-N-CA	-7.18	103.75	121.70
1	A	54	ARG	CD-NE-CZ	7.09	133.53	123.60
1	L	52	GLU	CG-CD-OE1	6.78	131.86	118.30
4	C	130	LYS	CG-CD-CE	6.71	132.03	111.90
5	F	65	LYS	N-CA-CB	6.70	122.66	110.60
2	H	193	PRO	N-CD-CG	-6.27	93.79	103.20
1	A	54	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	A	127	LEU	CB-CG-CD1	5.43	120.24	111.00
5	F	65	LYS	C-N-CA	-5.34	111.09	122.30
5	D	54	THR	C-N-CA	-5.26	111.26	122.30
3	G	94	GLN	N-CA-CB	5.24	120.04	110.60
2	H	132	LEU	CA-CB-CG	5.07	126.96	115.30
1	A	54	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	54	ARG	Sidechain
5	F	65	LYS	Peptide
5	F	87	ARG	Sidechain
3	G	98	ARG	Sidechain
2	H	150	VAL	Peptide
2	H	62	GLN	Sidechain

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	1603	0	1553	81	0
1	L	1603	0	1553	47	0
2	B	1616	0	1568	57	0
2	H	1651	0	1601	64	0
3	G	786	0	744	30	0
3	I	779	0	740	35	0
4	C	1556	0	1500	85	0
4	E	1596	0	1535	37	0
5	D	1551	0	1521	92	0
5	F	1626	0	1605	98	0
6	A	4	3	3	1	0
6	L	4	3	3	2	0
7	A	12	0	0	1	0
7	B	17	0	0	2	1
7	C	14	0	0	0	0
7	D	6	0	0	0	0
7	E	34	0	0	6	1
7	F	9	0	0	1	0
7	G	2	0	0	0	0
7	H	37	0	0	7	0
7	I	3	0	0	0	0
7	L	15	0	0	2	0
All	All	14524	6	13926	590	1

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 (590) 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:33:ARG:NH1	3:I:99:GLU:OE2	1.70	1.24
2:B:192:VAL:HG21	2:B:202:TYR:OH	1.40	1.21
4:C:32:TYR:HA	4:C:51:THR:OG1	1.50	1.11
2:H:143:THR:N	2:H:194:SER:HG	1.50	1.09
4:C:52:ASN:HB2	4:C:64:GLY:HA3	1.10	1.06
1:A:124:ASP:HA	1:A:127:LEU:HB2	1.02	1.02
4:C:48:ILE:CG2	4:C:52:ASN:HA	1.89	1.02
4:C:52:ASN:HB2	4:C:64:GLY:CA	1.91	1.01
5:D:163:ASN:OD1	5:D:205:ASN:ND2	1.94	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:166:ALA:HA	5:D:169:SER:HB3	1.43	0.99
1:L:32:ARG:NH2	1:L:52:GLU:OE1	1.96	0.99
2:B:192:VAL:HG23	2:B:193:PRO:HD2	1.45	0.98
4:C:128:ALA:O	4:C:130:LYS:HG3	1.66	0.96
3:I:49:THR:O	3:I:50:ARG:HD3	1.65	0.95
2:H:1:GLN:HA	2:H:1:GLN:NE2	1.80	0.95
1:A:151:LYS:HG2	1:A:156:LEU:HD23	1.50	0.94
2:H:137:LYS:HD2	2:H:137:LYS:O	1.66	0.94
2:H:143:THR:N	2:H:194:SER:OG	2.00	0.93
4:C:48:ILE:HG21	4:C:52:ASN:HA	1.48	0.93
1:A:124:ASP:CA	1:A:127:LEU:HB2	1.98	0.93
2:H:91:THR:HG22	2:H:119:VAL:HG13	1.46	0.93
5:D:173:THR:HG22	5:D:188:SER:OG	1.68	0.92
4:E:43:SER:OG	5:F:113:GLN:NE2	2.02	0.92
1:A:192:LYS:HE2	1:A:212:ASN:CG	1.89	0.92
5:F:154:PHE:HB3	5:F:155:PRO:HD3	1.49	0.92
5:F:192:VAL:HG21	5:F:202:TYR:OH	1.70	0.92
5:D:1:GLN:OE1	5:D:1:GLN:N	2.05	0.90
5:F:203:ILE:HD12	5:F:203:ILE:O	1.69	0.90
1:A:124:ASP:HA	1:A:127:LEU:CB	1.97	0.90
2:B:197:LEU:HD23	2:B:198:GLY:H	1.34	0.89
2:H:192:VAL:HB	2:H:193:PRO:HD3	1.55	0.88
5:F:192:VAL:HG23	5:F:193:PRO:HD2	1.56	0.88
1:A:145:GLU:OE1	1:A:145:GLU:N	2.05	0.88
1:A:125:GLU:OE1	1:A:128:LYS:NZ	2.07	0.87
4:E:31:ARG:O	7:E:301:HOH:O	1.91	0.87
1:L:200:HIS:ND1	1:L:201:GLN:O	2.07	0.86
5:D:12:VAL:HG21	5:D:18:LEU:HD22	1.58	0.85
5:F:220:GLU:CD	5:F:221:PRO:HD2	1.98	0.85
5:F:11:LEU:HD12	5:F:124:THR:HG22	1.58	0.84
3:I:14:CYS:O	3:I:18:VAL:HG12	1.77	0.84
4:C:133:LEU:HD12	4:C:181:LEU:HD11	1.59	0.83
1:L:145:GLU:N	1:L:145:GLU:OE2	2.12	0.83
3:I:12:MET:HB3	3:I:17:GLN:HG3	1.59	0.83
4:C:52:ASN:CB	4:C:64:GLY:HA3	2.03	0.82
1:A:123:SER:O	1:A:127:LEU:HD23	1.80	0.82
4:C:134:VAL:HG12	4:C:136:LEU:CD2	2.10	0.82
4:C:133:LEU:CD1	4:C:181:LEU:HD11	2.09	0.82
4:C:136:LEU:HD12	5:D:174:PHE:CE2	2.14	0.81
5:D:145:ALA:HB2	5:D:191:THR:HG22	1.61	0.81
2:B:1:GLN:N	2:B:1:GLN:OE1	2.14	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:133:LEU:HD12	4:E:181:LEU:HD11	1.61	0.81
5:F:208:HIS:HD1	5:F:211:SER:HG	1.26	0.81
5:D:203:ILE:O	5:D:203:ILE:HD12	1.79	0.81
5:F:88:ALA:HA	5:F:119:VAL:CG2	2.11	0.80
1:L:142:TYR:CD1	1:L:143:PRO:HA	2.16	0.80
4:E:212:CYS:SG	5:F:222:LYS:HE3	2.20	0.80
1:A:134:VAL:HG12	1:A:181:LEU:HB3	1.64	0.79
3:I:31:MET:HE3	3:I:31:MET:HA	1.63	0.79
5:D:166:ALA:HA	5:D:169:SER:CB	2.13	0.79
1:A:149:GLN:HE21	1:A:156:LEU:HD13	1.46	0.79
5:D:171:VAL:HG12	5:D:190:VAL:HG23	1.64	0.78
5:F:11:LEU:CD1	5:F:124:THR:HG22	2.12	0.78
1:A:144:ARG:HG2	1:A:144:ARG:HH11	1.48	0.78
2:H:192:VAL:HB	2:H:193:PRO:CD	2.14	0.78
1:L:185:LYS:O	1:L:189:GLU:HG2	1.84	0.77
1:A:117:VAL:HG21	1:A:198:VAL:HG21	1.64	0.77
5:F:173:THR:HG23	5:F:188:SER:OG	1.84	0.77
1:L:149:GLN:OE1	1:L:156:LEU:HD22	1.84	0.76
1:L:13:VAL:CG2	1:L:78:VAL:HG11	2.15	0.76
2:B:207:ASN:OD1	2:B:214:LYS:HG2	1.84	0.76
7:E:305:HOH:O	5:F:43:LYS:HB3	1.86	0.76
1:A:138:LEU:HD11	1:A:198:VAL:HG11	1.67	0.76
2:H:88:PRO:O	2:H:91:THR:HG23	1.87	0.75
5:D:150:VAL:CG2	5:D:186:LEU:HG	2.16	0.75
2:H:29:PHE:HA	7:H:303:HOH:O	1.87	0.75
4:C:134:VAL:HG12	4:C:136:LEU:HD22	1.68	0.74
1:A:134:VAL:CG1	1:A:181:LEU:HB3	2.17	0.74
1:A:168:GLN:HE21	1:A:173:SER:HB3	1.52	0.74
2:H:32:TYR:HB2	2:H:98:ARG:HD3	1.70	0.74
3:G:65:MET:O	3:G:68:THR:HG22	1.87	0.74
2:H:207:ASN:ND2	2:H:214:LYS:HD3	2.02	0.74
5:D:208:HIS:NE2	5:D:210:PRO:HG2	2.03	0.73
3:G:37:GLU:O	3:G:37:GLU:HG2	1.88	0.73
5:D:202:TYR:HB2	5:D:219:VAL:CG2	2.19	0.73
5:F:150:VAL:CG2	5:F:186:LEU:HG	2.18	0.72
2:H:30:THR:N	7:H:303:HOH:O	2.13	0.72
1:A:51:ASP:O	1:A:52:GLU:HB2	1.88	0.72
1:A:13:VAL:CG1	1:A:78:VAL:HG11	2.19	0.72
5:F:87:ARG:C	5:F:119:VAL:HG21	2.10	0.72
5:F:13:LYS:CG	5:F:14:PRO:HD2	2.20	0.71
5:D:88:ALA:O	5:D:91:THR:HG23	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:185:LYS:HD3	1:L:186:ALA:H	1.55	0.71
4:C:187:LYS:HA	4:C:187:LYS:HE2	1.73	0.70
5:D:12:VAL:HG21	5:D:18:LEU:CD2	2.20	0.70
2:H:98:ARG:HD2	2:H:99:SER:O	1.91	0.70
2:B:11:VAL:HG21	2:B:155:PRO:HG3	1.72	0.70
4:C:136:LEU:HD12	5:D:174:PHE:CZ	2.26	0.70
5:D:192:VAL:HG22	5:D:193:PRO:HD2	1.73	0.70
1:L:199:THR:HG22	1:L:206:PRO:HG3	1.74	0.70
4:E:124:GLU:N	4:E:124:GLU:OE2	2.23	0.70
3:G:70:GLY:O	3:G:71:CYS:HB2	1.92	0.70
5:F:30:SER:OG	7:F:301:HOH:O	2.08	0.70
5:F:150:VAL:HG22	5:F:186:LEU:HG	1.72	0.70
3:G:88:GLN:HA	3:G:88:GLN:OE1	1.90	0.70
4:C:58:ILE:HG23	4:C:59:PRO:HD2	1.74	0.69
2:H:91:THR:HG22	2:H:119:VAL:CG1	2.21	0.69
5:F:220:GLU:CG	5:F:221:PRO:HD2	2.22	0.69
5:D:160:VAL:HG22	5:D:206:VAL:HG12	1.74	0.68
2:H:1:GLN:HA	2:H:1:GLN:HE21	1.58	0.68
5:F:6:GLU:OE1	5:F:115:THR:HG23	1.93	0.68
1:A:126:GLN:O	1:A:129:SER:OG	2.08	0.68
4:C:119:PHE:CD2	5:D:132:LEU:HD22	2.29	0.67
3:I:99:GLU:OE1	3:I:99:GLU:HA	1.92	0.67
1:A:153:ASP:OD2	1:A:191:HIS:ND1	2.28	0.67
2:H:139:THR:O	2:H:194:SER:HB3	1.95	0.67
2:H:31:ASP:OD1	7:H:302:HOH:O	2.12	0.67
2:B:192:VAL:HG23	2:B:193:PRO:CD	2.23	0.67
3:I:34:ILE:HG13	3:I:35:MET:HG3	1.77	0.67
5:F:12:VAL:HG12	5:F:119:VAL:HG12	1.77	0.66
1:A:203:LEU:HD13	1:A:207:VAL:HG23	1.75	0.66
2:B:116:LEU:HD22	2:B:157:PRO:HD3	1.77	0.66
5:F:112:SER:O	5:F:113:GLN:HG2	1.94	0.66
5:D:34:MET:HB2	5:D:79:LEU:HD13	1.77	0.66
3:G:23:LEU:HD13	3:G:79:ILE:HG13	1.78	0.66
1:L:13:VAL:HG21	1:L:78:VAL:HG11	1.77	0.66
1:L:110:ARG:HG2	1:L:111:THR:N	2.11	0.66
2:B:192:VAL:CG2	2:B:193:PRO:HD2	2.24	0.65
5:D:150:VAL:HG22	5:D:186:LEU:HG	1.76	0.65
5:D:171:VAL:HG12	5:D:190:VAL:CG2	2.25	0.65
4:E:107:LEU:O	7:E:302:HOH:O	2.13	0.65
1:A:124:ASP:O	1:A:128:LYS:HG3	1.97	0.65
5:F:13:LYS:HG3	5:F:14:PRO:HD2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:91:TRP:CZ2	3:G:114:ARG:HB3	2.32	0.65
5:F:192:VAL:CG2	5:F:193:PRO:HD2	2.27	0.65
1:L:115:PRO:HB3	1:L:141:PHE:HB3	1.79	0.64
4:E:133:LEU:CD1	4:E:181:LEU:HD11	2.27	0.64
1:A:152:VAL:HG12	1:A:157:GLN:HG2	1.78	0.64
2:B:172:HIS:HE1	1:A:140:ASN:OD1	1.81	0.64
2:B:124:THR:CG2	2:B:211:SER:HB3	2.28	0.64
1:A:13:VAL:HG11	1:A:78:VAL:HG11	1.78	0.63
2:B:13:LYS:HD3	2:B:121:SER:HA	1.81	0.63
2:B:192:VAL:CG2	2:B:202:TYR:OH	2.33	0.63
3:G:91:GLN:HA	3:G:94:GLN:OE1	1.99	0.63
4:C:128:ALA:C	4:C:130:LYS:HG3	2.17	0.63
5:D:163:ASN:OD1	5:D:205:ASN:CG	2.37	0.63
2:B:98:ARG:NH2	7:B:302:HOH:O	2.31	0.63
1:A:157:GLN:HB3	1:A:160:ASN:HD21	1.63	0.62
5:D:60:TYR:CD1	5:D:68:LEU:HD12	2.34	0.62
3:G:63:ASN:HA	3:G:68:THR:HG21	1.81	0.62
5:D:171:VAL:CG1	5:D:190:VAL:HG23	2.29	0.62
2:H:32:TYR:CB	2:H:98:ARG:HD3	2.29	0.62
4:C:116:VAL:O	4:C:205:LYS:HE2	1.99	0.62
1:L:5:LEU:HD11	1:L:90:VAL:HG13	1.80	0.62
2:B:197:LEU:HD23	2:B:198:GLY:N	2.12	0.62
4:C:5:LEU:HD11	4:C:90:THR:HG22	1.81	0.62
4:C:33:VAL:H	4:C:51:THR:HA	1.63	0.62
5:F:220:GLU:OE1	5:F:221:PRO:HD2	2.00	0.62
2:B:197:LEU:CD2	2:B:198:GLY:H	2.11	0.62
4:C:116:VAL:O	4:C:205:LYS:CE	2.48	0.62
2:B:124:THR:HG22	2:B:211:SER:HB3	1.81	0.62
5:F:12:VAL:CG1	5:F:119:VAL:HG12	2.29	0.62
3:I:31:MET:HA	3:I:31:MET:CE	2.29	0.61
1:A:58:ILE:HG13	1:A:58:ILE:O	2.00	0.61
2:H:152:ASP:N	7:H:301:HOH:O	1.87	0.61
4:C:13:VAL:HG22	4:C:17:GLN:HB2	1.81	0.61
3:G:34:ILE:HG13	3:G:35:MET:N	2.14	0.61
2:H:192:VAL:CB	2:H:193:PRO:CD	2.78	0.61
1:A:152:VAL:CG1	1:A:157:GLN:HG2	2.30	0.61
5:F:1:GLN:OE1	5:F:1:GLN:N	2.28	0.61
1:L:60:ASP:OD1	1:L:62:PHE:N	2.25	0.61
4:C:72:THR:HG22	4:C:74:THR:HG22	1.83	0.61
3:I:34:ILE:O	3:I:35:MET:HB2	2.01	0.60
2:H:104:GLU:OE1	2:H:104:GLU:N	2.25	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:161:SER:O	2:H:204:CYS:O	2.19	0.60
2:B:94:TYR:CD1	2:B:117:VAL:HG13	2.36	0.60
5:D:147:GLY:HA2	5:D:162:TRP:HH2	1.65	0.60
5:D:73:ASP:OD1	5:D:76:LYS:HB2	2.02	0.60
4:E:133:LEU:HD12	4:E:181:LEU:CD1	2.31	0.60
1:L:152:VAL:HG12	1:L:194:TYR:CD2	2.37	0.60
5:F:64:MET:O	5:F:65:LYS:C	2.38	0.60
5:D:166:ALA:CA	5:D:169:SER:HB3	2.27	0.60
3:G:23:LEU:O	3:G:27:GLU:HG3	2.02	0.59
1:A:151:LYS:CG	1:A:156:LEU:HD23	2.29	0.59
3:G:86:ARG:HD3	4:C:54:ARG:NE	2.17	0.59
2:B:11:VAL:CG2	2:B:155:PRO:HG3	2.31	0.59
3:I:18:VAL:HA	3:I:65:MET:HE3	1.84	0.59
4:C:79:GLN:HB2	4:C:81:LEU:CD2	2.33	0.59
2:H:169:SER:O	7:H:304:HOH:O	2.17	0.59
4:C:34:SER:HB3	4:C:89:LEU:HB3	1.85	0.59
5:D:203:ILE:HA	5:D:217:LYS:O	2.03	0.59
4:C:49:TYR:HE1	4:C:55:PRO:O	1.85	0.58
2:B:4:LEU:O	7:B:301:HOH:O	2.17	0.58
1:A:188:TYR:HA	1:A:194:TYR:OH	2.04	0.58
2:H:87:THR:O	2:H:119:VAL:HG11	2.04	0.58
2:H:27:TYR:CD1	2:H:98:ARG:NH1	2.71	0.58
2:B:175:PRO:HG2	1:A:164:SER:OG	2.04	0.58
4:E:150:LYS:HE2	4:E:195:GLN:OE1	2.03	0.58
4:C:48:ILE:HG22	4:C:52:ASN:HA	1.85	0.58
4:C:51:THR:HG22	4:C:51:THR:O	2.04	0.58
1:A:153:ASP:OD1	1:A:191:HIS:HB3	2.03	0.58
4:E:47:VAL:HG12	4:E:58:ILE:HD12	1.85	0.58
5:F:29:PHE:O	5:F:30:SER:OG	2.12	0.58
4:C:14:SER:HB2	4:C:17:GLN:OE1	2.04	0.58
5:D:192:VAL:HG11	5:D:202:TYR:OH	2.03	0.58
1:L:185:LYS:HD3	1:L:186:ALA:N	2.18	0.57
4:C:52:ASN:OD1	4:C:65:SER:N	2.37	0.57
5:F:112:SER:C	5:F:113:GLN:HG2	2.22	0.57
1:A:151:LYS:HB2	1:A:195:ALA:HB3	1.86	0.57
3:I:84:CYS:HA	3:I:87:LEU:HD12	1.85	0.57
4:C:192:TYR:O	4:C:206:THR:HG23	2.05	0.57
5:F:13:LYS:HG2	5:F:14:PRO:HD2	1.86	0.57
4:C:133:LEU:HD11	4:C:181:LEU:HD11	1.87	0.57
5:F:131:PRO:HD3	5:F:217:LYS:HE3	1.87	0.57
5:F:220:GLU:OE1	5:F:220:GLU:HA	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ARG:HG2	1:A:111:THR:N	2.20	0.57
4:C:96:PRO:HG2	5:D:47:TRP:CG	2.40	0.56
5:F:15:GLY:N	5:F:86:LEU:O	2.24	0.56
3:G:82:ASN:OD1	5:D:101:PHE:HB3	2.05	0.56
1:L:62:PHE:CE2	1:L:75:ILE:HG12	2.40	0.56
5:F:205:ASN:HB3	5:F:216:ASP:OD1	2.06	0.56
5:F:220:GLU:HG3	5:F:221:PRO:HD2	1.87	0.56
4:C:128:ALA:O	4:C:130:LYS:CG	2.47	0.56
1:L:25:ALA:HB3	1:L:28:ILE:HD12	1.88	0.56
2:B:147:GLY:HA2	2:B:162:TRP:CZ2	2.40	0.56
4:C:119:PHE:CE2	5:D:132:LEU:HB3	2.39	0.56
4:E:5:LEU:HD11	4:E:90:THR:HG22	1.88	0.56
5:D:202:TYR:O	5:D:219:VAL:HG22	2.04	0.56
1:A:131:THR:HG22	1:A:132:ALA:N	2.22	0.56
5:D:163:ASN:ND2	5:D:203:ILE:HD13	2.21	0.55
5:D:192:VAL:HG11	5:D:202:TYR:CZ	2.41	0.55
2:H:91:THR:HB	2:H:118:THR:HA	1.88	0.55
1:A:192:LYS:HE2	1:A:212:ASN:OD1	2.04	0.55
1:L:110:ARG:NH1	1:L:111:THR:HG23	2.22	0.55
5:D:12:VAL:O	5:D:119:VAL:HA	2.07	0.55
1:L:13:VAL:HG23	1:L:78:VAL:HG11	1.87	0.55
2:H:1:GLN:NE2	2:H:1:GLN:CA	2.58	0.55
1:A:115:PRO:HB3	1:A:141:PHE:HB3	1.87	0.55
4:C:134:VAL:HG12	4:C:136:LEU:HD21	1.85	0.55
4:E:101:GLY:N	7:E:303:HOH:O	2.26	0.55
4:E:43:SER:CB	5:F:113:GLN:NE2	2.70	0.55
2:H:10:ASP:O	2:H:117:VAL:HA	2.06	0.55
3:G:12:MET:CE	3:G:16:ARG:HD3	2.37	0.55
5:D:166:ALA:CA	5:D:169:SER:CB	2.83	0.55
5:F:12:VAL:O	5:F:119:VAL:HA	2.07	0.55
1:A:21:ILE:HD12	1:A:73:LEU:HD23	1.89	0.54
4:E:43:SER:H	5:F:113:GLN:HE22	1.53	0.54
2:H:85:GLY:O	7:H:305:HOH:O	2.18	0.54
5:D:166:ALA:C	5:D:169:SER:HB2	2.27	0.54
2:H:1:GLN:HG3	2:H:2:VAL:H	1.73	0.54
5:D:94:TYR:CE1	5:D:117:VAL:HG22	2.43	0.54
1:A:151:LYS:HG2	1:A:156:LEU:CD2	2.30	0.54
1:A:196:CYS:O	1:A:208:THR:HA	2.07	0.54
2:B:116:LEU:HD23	2:B:116:LEU:O	2.07	0.54
4:E:87:TYR:OH	5:F:43:LYS:O	2.21	0.54
4:C:150:LYS:HB2	4:C:193:SER:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:GLN:NE2	1:A:173:SER:HB3	2.21	0.54
6:L:301:ACT:H2	7:L:401:HOH:O	2.08	0.54
5:D:218:LYS:HD2	5:D:219:VAL:N	2.23	0.54
4:E:157:LYS:HD3	4:E:158:ALA:H	1.71	0.53
2:B:47:TRP:CZ2	2:B:49:GLY:HA2	2.43	0.53
4:C:134:VAL:CG1	4:C:136:LEU:HD21	2.38	0.53
5:F:153:TYR:CE1	5:F:184:TYR:HB2	2.43	0.53
1:A:192:LYS:HB3	1:A:193:VAL:HG23	1.90	0.53
2:B:127:PRO:HB3	2:B:153:TYR:HB3	1.90	0.53
2:B:33:GLU:HG3	3:I:113:GLN:OE1	2.08	0.53
3:G:103:LEU:HB3	3:G:104:PRO:HD3	1.90	0.53
1:L:152:VAL:HG22	1:L:157:GLN:NE2	2.23	0.53
5:D:171:VAL:HG12	5:D:190:VAL:CB	2.39	0.53
3:G:84:CYS:HA	3:G:87:LEU:HD12	1.91	0.53
5:D:202:TYR:HB2	5:D:219:VAL:HG21	1.91	0.53
4:C:133:LEU:HD21	4:C:186:TRP:CZ3	2.44	0.53
1:A:124:ASP:OD1	1:A:124:ASP:N	2.41	0.53
1:A:144:ARG:HH11	1:A:144:ARG:CG	2.20	0.53
1:A:13:VAL:HG13	1:A:78:VAL:HG11	1.89	0.52
2:B:4:LEU:HD22	2:B:24:THR:HG22	1.91	0.52
4:C:47:VAL:O	4:C:48:ILE:HG12	2.09	0.52
4:C:137:ILE:HG12	4:C:196:VAL:HG21	1.91	0.52
1:L:212:ASN:O	1:L:213:ARG:HG2	2.09	0.52
4:C:157:LYS:H	4:C:157:LYS:HD3	1.75	0.52
5:D:53:ALA:HA	5:D:72:ARG:NH1	2.23	0.52
5:D:192:VAL:HG22	5:D:193:PRO:CD	2.38	0.52
4:C:119:PHE:HD2	5:D:132:LEU:HD22	1.74	0.52
4:C:190:ARG:HG3	4:C:190:ARG:HH11	1.75	0.52
5:D:208:HIS:CD2	5:D:210:PRO:HG2	2.43	0.52
3:G:12:MET:HE2	3:G:16:ARG:HD3	1.92	0.52
4:C:52:ASN:ND2	4:C:65:SER:O	2.43	0.52
5:D:40:ALA:HB3	5:D:43:LYS:HG2	1.92	0.52
5:D:202:TYR:HB2	5:D:219:VAL:HG22	1.92	0.52
4:E:100:THR:CA	7:E:303:HOH:O	2.58	0.52
5:F:53:ALA:HA	5:F:72:ARG:NH1	2.25	0.52
2:H:32:TYR:CD1	2:H:98:ARG:NH1	2.78	0.52
4:E:100:THR:HA	7:E:303:HOH:O	2.10	0.52
2:B:203:ILE:HG12	2:B:218:LYS:HD2	1.92	0.52
2:H:4:LEU:HD22	2:H:24:THR:HG22	1.92	0.51
4:C:51:THR:O	4:C:52:ASN:OD1	2.28	0.51
4:C:136:LEU:HD12	5:D:174:PHE:CD2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:13:LYS:HG3	5:F:14:PRO:CD	2.39	0.51
5:F:203:ILE:HD12	5:F:203:ILE:C	2.30	0.51
3:I:12:MET:SD	3:I:16:ARG:HG2	2.50	0.51
3:I:17:GLN:OE1	3:I:66:GLU:N	2.43	0.51
3:I:49:THR:O	3:I:50:ARG:CD	2.50	0.51
5:F:127:PRO:HB3	5:F:153:TYR:HB3	1.93	0.51
4:C:157:LYS:HD3	4:C:158:ALA:H	1.74	0.51
5:F:154:PHE:CB	5:F:155:PRO:HD3	2.30	0.51
3:G:89:ASP:CB	3:G:92:MET:HE2	2.41	0.51
3:I:49:THR:C	3:I:50:ARG:HD3	2.29	0.51
4:C:52:ASN:O	4:C:64:GLY:CA	2.58	0.51
5:D:163:ASN:HD21	5:D:203:ILE:HD13	1.74	0.51
5:D:94:TYR:CE1	5:D:117:VAL:CG2	2.93	0.51
5:F:94:TYR:CE1	5:F:117:VAL:HG22	2.46	0.51
2:H:60:TYR:CE1	2:H:70:MET:HG3	2.46	0.51
3:I:114:ARG:HB3	1:A:91:TRP:CZ2	2.46	0.51
3:G:89:ASP:HB2	3:G:92:MET:HE2	1.93	0.51
2:B:34:MET:SD	2:B:98:ARG:HG2	2.51	0.50
5:D:217:LYS:HE3	5:D:217:LYS:HA	1.93	0.50
1:A:167:GLU:OE1	1:A:167:GLU:HA	2.11	0.50
3:I:99:GLU:OE1	3:I:99:GLU:CA	2.59	0.50
2:B:116:LEU:CD2	2:B:157:PRO:HD3	2.42	0.50
3:I:34:ILE:O	3:I:35:MET:CB	2.59	0.50
2:H:207:ASN:HD22	2:H:214:LYS:HD3	1.72	0.50
2:B:130:PHE:HB3	1:A:123:SER:OG	2.12	0.50
4:E:16:GLY:O	4:E:77:GLY:HA2	2.11	0.50
1:A:6:THR:HA	7:A:401:HOH:O	2.11	0.50
1:A:31:LYS:O	1:A:66:LYS:HE3	2.11	0.50
2:B:134:PRO:HB3	2:B:145:ALA:O	2.11	0.50
2:H:47:TRP:CZ2	2:H:49:GLY:HA2	2.47	0.50
3:G:12:MET:HG3	3:G:17:GLN:HG3	1.94	0.50
5:F:88:ALA:HA	5:F:119:VAL:HG23	1.94	0.50
1:A:53:ASP:HB3	1:A:54:ARG:HD3	1.93	0.50
1:L:32:ARG:HH12	1:L:52:GLU:CD	2.14	0.49
2:B:62:GLN:HG3	2:B:63:LYS:N	2.25	0.49
4:C:53:GLN:HB2	4:C:54:ARG:NH1	2.27	0.49
4:C:187:LYS:HA	4:C:187:LYS:CE	2.34	0.49
5:D:150:VAL:HG21	5:D:186:LEU:HG	1.92	0.49
1:L:120:PHE:CB	2:H:132:LEU:HD12	2.42	0.49
5:F:11:LEU:HD12	5:F:124:THR:CG2	2.37	0.49
1:L:39:LYS:HB3	1:L:40:PRO:CD	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:218:LYS:HD2	5:D:219:VAL:O	2.12	0.49
5:F:143:THR:CA	5:F:194:SER:HB2	2.42	0.49
5:D:209:LYS:N	5:D:210:PRO:HD2	2.27	0.49
5:D:152:ASP:HB3	5:D:183:LEU:HD13	1.93	0.49
5:D:218:LYS:HD2	5:D:219:VAL:H	1.77	0.49
3:I:90:ARG:HA	3:I:93:VAL:HB	1.94	0.49
5:D:94:TYR:HE1	5:D:117:VAL:HG22	1.76	0.49
1:A:12:SER:HB3	1:A:109:LEU:HD21	1.95	0.49
1:A:53:ASP:O	1:A:54:ARG:HD2	2.11	0.49
2:H:49:GLY:HA3	2:H:70:MET:HE3	1.93	0.49
5:D:164:SER:C	5:D:166:ALA:N	2.64	0.49
2:H:12:ARG:O	2:H:119:VAL:HA	2.13	0.49
2:B:11:VAL:HG22	2:B:118:THR:HB	1.94	0.49
3:G:67:ASN:O	3:G:70:GLY:O	2.31	0.49
4:C:49:TYR:CE1	4:C:55:PRO:O	2.66	0.49
4:C:119:PHE:CD2	5:D:132:LEU:HB3	2.48	0.49
1:A:117:VAL:CG2	1:A:198:VAL:HG21	2.40	0.49
4:C:33:VAL:H	4:C:51:THR:CA	2.25	0.48
5:D:163:ASN:ND2	5:D:203:ILE:CD1	2.75	0.48
4:E:96:PRO:HG2	5:F:47:TRP:CG	2.49	0.48
2:H:1:GLN:HE21	2:H:1:GLN:CA	2.22	0.48
3:G:103:LEU:HD12	3:G:103:LEU:O	2.13	0.48
5:D:68:LEU:HD13	5:D:81:LEU:HD11	1.95	0.48
5:F:150:VAL:HG23	5:F:150:VAL:O	2.13	0.48
2:B:192:VAL:CG2	2:B:193:PRO:CD	2.88	0.48
1:L:110:ARG:O	1:L:142:TYR:HE2	1.96	0.48
1:A:194:TYR:O	1:A:210:SER:HA	2.13	0.48
5:D:83:MET:HB3	5:D:86:LEU:HD21	1.94	0.48
6:L:301:ACT:C	7:L:401:HOH:O	2.62	0.48
2:H:60:TYR:HE1	2:H:70:MET:HG3	1.78	0.48
3:I:31:MET:CE	3:I:31:MET:CA	2.91	0.48
5:D:17:SER:OG	5:D:84:ASN:ND2	2.45	0.48
1:A:136:CYS:HB2	1:A:150:TRP:CZ2	2.49	0.48
1:L:60:ASP:OD1	1:L:60:ASP:C	2.52	0.48
3:I:23:LEU:HD13	3:I:79:ILE:HG13	1.96	0.48
4:C:133:LEU:HD13	4:C:179:LEU:HD23	1.96	0.47
5:D:127:PRO:HB3	5:D:153:TYR:HB3	1.95	0.47
1:L:19:ALA:O	1:L:74:THR:HA	2.14	0.47
5:F:68:LEU:HA	5:F:82:GLN:O	2.14	0.47
1:L:151:LYS:HA	1:L:155:ALA:O	2.14	0.47
3:G:53:ASP:O	3:G:57:ARG:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:28:THR:O	5:F:31:ASP:HB2	2.14	0.47
2:H:65:GLN:HG3	7:H:306:HOH:O	2.13	0.47
2:B:18:VAL:HB	2:B:86:LEU:HD11	1.97	0.47
5:F:194:SER:O	5:F:197:LEU:HD23	2.15	0.47
4:C:145:VAL:HG12	4:C:198:HIS:HB2	1.96	0.47
1:A:134:VAL:CG2	1:A:211:PHE:HE2	2.27	0.47
4:C:188:SER:OG	4:C:189:HIS:ND1	2.45	0.47
5:D:60:TYR:CD1	5:D:68:LEU:CD1	2.98	0.47
5:D:207:ASN:ND2	5:D:214:LYS:HG2	2.28	0.47
5:F:99:ARG:HA	5:F:107:ILE:O	2.15	0.47
2:B:101:GLY:O	3:I:113:GLN:HG2	2.14	0.47
4:E:167:LYS:HG3	4:E:173:TYR:CE2	2.50	0.47
5:F:94:TYR:HE1	5:F:117:VAL:HG22	1.80	0.47
5:F:96:CYS:HB3	5:F:112:SER:HB3	1.97	0.47
2:B:178:LEU:HD21	2:B:182:GLY:HA2	1.96	0.46
3:I:66:GLU:HG2	3:I:67:ASN:ND2	2.30	0.46
1:L:167:GLU:HA	1:L:167:GLU:OE1	2.14	0.46
2:H:161:SER:OG	2:H:205:ASN:HB2	2.16	0.46
5:D:105:SER:O	5:D:107:ILE:HG23	2.15	0.46
1:A:13:VAL:HG21	1:A:19:ALA:HB2	1.96	0.46
2:H:52:ASN:OD1	2:H:54:HIS:N	2.48	0.46
2:H:156:GLU:O	2:H:156:GLU:OE1	2.32	0.46
3:G:16:ARG:HG3	5:D:57:ASN:OD1	2.15	0.46
3:I:89:ASP:OD2	3:I:91:GLN:N	2.48	0.46
2:H:1:GLN:CG	2:H:2:VAL:H	2.27	0.46
2:H:125:LYS:HD3	2:H:152:ASP:O	2.16	0.46
5:F:13:LYS:CG	5:F:14:PRO:CD	2.92	0.46
3:G:70:GLY:O	3:G:71:CYS:CB	2.59	0.46
5:F:155:PRO:HB2	5:F:210:PRO:CB	2.46	0.46
2:B:76:ASP:O	2:B:78:THR:HG22	2.16	0.46
5:F:83:MET:HB3	5:F:86:LEU:HD21	1.97	0.46
5:F:124:THR:HB	5:F:155:PRO:HG2	1.97	0.46
2:H:50:LEU:HD12	2:H:50:LEU:C	2.36	0.46
4:C:122:SER:O	4:C:126:LEU:HD12	2.16	0.46
1:L:110:ARG:HG2	1:L:111:THR:H	1.79	0.46
2:H:218:LYS:CD	2:H:218:LYS:H	2.29	0.46
5:D:150:VAL:HG22	5:D:186:LEU:O	2.15	0.46
1:L:23:CYS:HB2	1:L:35:TRP:CH2	2.51	0.46
3:I:13:SER:O	3:I:17:GLN:HB2	2.16	0.45
4:E:37:GLN:HB2	4:E:86:TYR:CE2	2.51	0.45
3:G:29:HIS:CD2	3:G:55:GLN:HB2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:191:SER:HB2	4:C:206:THR:CG2	2.46	0.45
1:A:40:PRO:HG3	1:A:167:GLU:HG3	1.98	0.45
2:H:167:LEU:HD21	2:H:190:VAL:HG21	1.98	0.45
4:C:52:ASN:OD1	4:C:65:SER:CA	2.64	0.45
4:E:165:PRO:HA	4:E:174:ALA:O	2.16	0.45
1:A:138:LEU:HD11	1:A:198:VAL:CG1	2.39	0.45
1:A:168:GLN:HG2	1:A:173:SER:HA	1.98	0.45
5:F:83:MET:CB	5:F:86:LEU:HD21	2.47	0.45
5:F:96:CYS:HB3	5:F:112:SER:CB	2.47	0.45
5:F:169:SER:OG	5:F:170:GLY:N	2.49	0.45
4:C:49:TYR:HB2	5:D:107:ILE:HG21	1.99	0.45
4:C:51:THR:HG21	4:C:66:ASP:OD2	2.17	0.45
4:C:168:GLN:HG2	5:D:172:HIS:CD2	2.51	0.45
1:A:149:GLN:HG2	1:A:156:LEU:CD2	2.47	0.45
3:I:55:GLN:O	3:I:58:CYS:HB3	2.17	0.45
4:C:18:THR:HB	4:C:76:SER:HA	1.97	0.45
2:H:116:LEU:HD23	2:H:157:PRO:HB3	1.99	0.45
2:H:218:LYS:H	2:H:218:LYS:CE	2.30	0.45
3:I:56:GLN:NE2	3:I:60:ASP:OD1	2.49	0.45
5:F:68:LEU:O	5:F:68:LEU:HD12	2.15	0.45
4:C:53:GLN:H	4:C:53:GLN:HG2	1.55	0.45
5:F:192:VAL:CG2	5:F:193:PRO:CD	2.94	0.45
1:A:31:LYS:HE3	1:A:92:ASP:HA	1.98	0.45
2:B:94:TYR:CE1	2:B:117:VAL:HG13	2.52	0.45
5:F:208:HIS:ND1	5:F:211:SER:OG	2.34	0.45
2:H:4:LEU:CD2	2:H:24:THR:HG22	2.46	0.45
5:D:19:ARG:HH11	5:D:19:ARG:HG3	1.82	0.45
5:D:174:PHE:CD2	5:D:174:PHE:N	2.85	0.45
5:F:34:MET:HB2	5:F:79:LEU:HD13	1.98	0.45
5:F:192:VAL:HG21	5:F:202:TYR:HH	1.74	0.45
1:L:37:ARG:HG3	1:L:86:TYR:CZ	2.51	0.44
2:H:220:GLU:HB2	2:H:221:PRO:HD2	1.98	0.44
5:F:214:LYS:HE2	5:F:214:LYS:HB3	1.57	0.44
1:L:161:SER:HA	1:L:180:THR:O	2.16	0.44
5:D:174:PHE:HE2	5:D:189:VAL:HG12	1.82	0.44
5:F:20:LEU:HD23	5:F:83:MET:CE	2.47	0.44
1:A:103:GLY:HA3	6:A:301:ACT:H3	1.99	0.44
3:I:89:ASP:OD2	3:I:89:ASP:C	2.56	0.44
4:E:166:SER:OG	5:F:175:PRO:HG2	2.17	0.44
5:F:119:VAL:HG23	5:F:119:VAL:O	2.17	0.44
1:A:192:LYS:HE2	1:A:212:ASN:ND2	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:27:TYR:CE1	2:H:98:ARG:NH1	2.86	0.44
2:B:10:ASP:O	2:B:117:VAL:HA	2.18	0.44
5:F:197:LEU:N	5:F:197:LEU:HD22	2.32	0.44
1:A:153:ASP:HA	1:A:193:VAL:HB	1.99	0.44
1:A:188:TYR:HH	1:A:211:PHE:HE1	1.65	0.44
4:C:79:GLN:HB2	4:C:81:LEU:HD23	1.98	0.44
5:F:87:ARG:O	5:F:119:VAL:HG21	2.18	0.44
1:A:110:ARG:HG2	1:A:111:THR:H	1.82	0.44
2:B:158:VAL:HG23	2:B:208:HIS:CD2	2.53	0.44
4:C:133:LEU:CD1	4:C:179:LEU:HD23	2.48	0.44
5:D:34:MET:CB	5:D:79:LEU:HD13	2.47	0.44
5:D:217:LYS:HA	5:D:217:LYS:CE	2.47	0.44
4:E:161:GLU:OE1	5:F:179:GLN:HA	2.18	0.44
5:F:87:ARG:O	5:F:90:ASP:HB2	2.18	0.44
1:L:193:VAL:HG22	1:L:212:ASN:OD1	2.17	0.44
2:H:137:LYS:O	2:H:137:LYS:CD	2.53	0.44
1:A:134:VAL:HG23	1:A:211:PHE:HE2	1.82	0.44
1:A:144:ARG:HG2	1:A:144:ARG:NH1	2.25	0.44
4:C:47:VAL:C	4:C:48:ILE:HG12	2.38	0.43
4:C:18:THR:HA	4:C:75:ILE:O	2.18	0.43
4:C:125:GLU:HA	5:D:130:PHE:CE1	2.53	0.43
1:A:53:ASP:C	1:A:54:ARG:CD	2.87	0.43
2:B:192:VAL:HG21	2:B:202:TYR:CZ	2.42	0.43
3:G:21:VAL:HG13	3:G:61:GLU:HB3	2.00	0.43
4:C:157:LYS:HD3	4:C:158:ALA:N	2.33	0.43
5:D:220:GLU:HG3	5:D:220:GLU:O	2.19	0.43
3:G:86:ARG:HD3	4:C:54:ARG:HE	1.82	0.43
4:E:157:LYS:HD3	4:E:158:ALA:N	2.33	0.43
5:F:94:TYR:CE1	5:F:117:VAL:CG2	3.01	0.43
2:B:40:ALA:HB3	2:B:43:GLN:HG3	1.99	0.43
1:A:61:ARG:HH11	1:A:61:ARG:HG3	1.84	0.43
1:L:115:PRO:CB	1:L:141:PHE:HB3	2.48	0.43
3:I:103:LEU:HB3	3:I:104:PRO:HD3	2.00	0.43
4:C:51:THR:C	4:C:52:ASN:CG	2.77	0.43
4:E:168:GLN:OE1	4:E:174:ALA:HB2	2.19	0.43
5:F:176:ALA:HB2	5:F:186:LEU:HB3	2.00	0.43
1:A:144:ARG:CG	1:A:144:ARG:NH1	2.80	0.43
2:B:116:LEU:HD23	2:B:116:LEU:C	2.38	0.43
3:G:55:GLN:O	3:G:58:CYS:HB3	2.19	0.43
5:F:65:LYS:O	5:F:67:ARG:N	2.52	0.43
1:L:110:ARG:HH12	1:L:111:THR:HG23	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:218:LYS:HB3	2:H:218:LYS:HE3	1.91	0.43
2:B:171:VAL:HG22	2:B:190:VAL:HG23	2.01	0.43
3:I:90:ARG:O	3:I:94:GLN:OE1	2.37	0.43
5:F:150:VAL:CG2	5:F:150:VAL:O	2.66	0.43
2:B:147:GLY:HA2	2:B:162:TRP:CH2	2.53	0.43
3:I:117:LEU:HD23	3:I:117:LEU:HA	1.88	0.43
4:C:56:SER:C	4:C:58:ILE:H	2.22	0.43
2:B:129:VAL:HG22	2:B:150:VAL:HG22	2.00	0.43
5:D:43:LYS:HD3	5:D:43:LYS:N	2.34	0.43
5:D:91:THR:HB	5:D:118:THR:HA	2.00	0.43
5:F:159:THR:OG1	5:F:207:ASN:HB3	2.18	0.43
2:B:98:ARG:HD2	2:B:98:ARG:C	2.38	0.42
2:B:172:HIS:CE1	1:A:140:ASN:OD1	2.67	0.42
3:I:31:MET:HE3	3:I:31:MET:CA	2.41	0.42
4:C:184:GLU:O	4:C:188:SER:HB3	2.19	0.42
4:E:151:ALA:HB2	4:E:192:TYR:CE2	2.53	0.42
5:F:162:TRP:CH2	5:F:204:CYS:HB3	2.53	0.42
1:A:25:ALA:HB3	1:A:28:ILE:HB	2.00	0.42
1:L:163:GLU:HA	1:L:178:SER:O	2.18	0.42
2:H:16:ALA:O	2:H:86:LEU:HG	2.19	0.42
4:E:167:LYS:HG3	4:E:173:TYR:CZ	2.54	0.42
2:H:132:LEU:HD21	2:H:149:LEU:HB2	2.02	0.42
4:E:154:SER:HB3	4:E:155:PRO:CD	2.49	0.42
5:F:168:THR:HG22	5:F:168:THR:O	2.20	0.42
5:D:150:VAL:HG23	5:D:150:VAL:O	2.19	0.42
1:A:133:SER:OG	1:A:182:THR:HG22	2.20	0.42
1:L:35:TRP:HA	1:L:87:TYR:O	2.20	0.42
4:C:51:THR:O	4:C:52:ASN:CG	2.58	0.42
5:F:203:ILE:HA	5:F:217:LYS:O	2.20	0.42
2:B:94:TYR:O	2:B:114:GLY:HA2	2.20	0.42
3:I:33:ARG:HD3	3:I:99:GLU:OE2	2.20	0.42
4:C:52:ASN:CG	4:C:65:SER:N	2.73	0.42
5:D:18:LEU:HD12	5:D:18:LEU:HA	1.91	0.42
4:E:161:GLU:OE1	5:F:180:SER:N	2.50	0.42
1:A:157:GLN:CB	1:A:160:ASN:HD21	2.31	0.42
5:D:166:ALA:C	5:D:169:SER:CB	2.87	0.42
3:G:24:LYS:N	3:G:25:PRO:HD2	2.34	0.42
4:C:48:ILE:HG21	4:C:52:ASN:CA	2.34	0.42
5:D:94:TYR:HE1	5:D:117:VAL:CG2	2.33	0.42
5:D:100:LYS:HG3	5:D:109:ASP:OD2	2.20	0.42
5:D:174:PHE:H	5:D:174:PHE:HD2	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:GLU:HA	1:A:128:LYS:NZ	2.35	0.42
1:A:187:ASP:O	1:A:190:LYS:HG2	2.20	0.42
1:A:194:TYR:O	1:A:210:SER:HB3	2.20	0.42
5:F:154:PHE:HB3	5:F:155:PRO:CD	2.35	0.41
1:L:120:PHE:HB2	2:H:132:LEU:HD12	2.00	0.41
2:B:76:ASP:OD1	2:B:78:THR:HG23	2.19	0.41
5:D:43:LYS:N	5:D:43:LYS:CD	2.83	0.41
5:D:99:ARG:HA	5:D:107:ILE:O	2.19	0.41
5:D:145:ALA:CB	5:D:191:THR:HG22	2.41	0.41
1:A:149:GLN:NE2	1:A:156:LEU:HD13	2.25	0.41
1:L:19:ALA:HB3	1:L:75:ILE:HB	2.02	0.41
5:D:99:ARG:HG3	5:D:108:PHE:CE1	2.54	0.41
1:L:117:VAL:O	1:L:209:LYS:HE2	2.21	0.41
1:L:164:SER:OG	2:H:175:PRO:HG2	2.20	0.41
2:H:94:TYR:CD1	2:H:117:VAL:HG13	2.56	0.41
4:E:124:GLU:HB2	5:F:130:PHE:HD1	1.85	0.41
4:E:135:CYS:HB2	4:E:149:TRP:CH2	2.56	0.41
5:F:161:SER:OG	5:F:205:ASN:ND2	2.53	0.41
2:H:91:THR:HA	2:H:117:VAL:O	2.21	0.41
4:E:183:PRO:O	4:E:186:TRP:HB3	2.21	0.41
2:B:116:LEU:HD22	2:B:157:PRO:CD	2.46	0.41
4:C:14:SER:HB2	4:C:17:GLN:CD	2.41	0.41
2:H:170:GLY:O	2:H:190:VAL:HA	2.21	0.41
2:B:177:VAL:CG1	1:A:162:GLN:OE1	2.69	0.41
4:C:123:SER:HA	4:C:126:LEU:HD12	2.02	0.41
4:C:136:LEU:HD22	4:C:136:LEU:N	2.36	0.41
5:F:11:LEU:HD23	5:F:118:THR:O	2.20	0.41
5:F:20:LEU:HD13	5:F:20:LEU:HA	1.91	0.41
5:F:88:ALA:CA	5:F:119:VAL:CG2	2.93	0.41
5:F:163:ASN:HB3	5:F:166:ALA:HB3	2.02	0.41
1:L:61:ARG:HH22	1:L:82:ASP:CG	2.24	0.40
4:E:136:LEU:HB3	5:F:174:PHE:CZ	2.55	0.40
5:F:132:LEU:N	5:F:147:GLY:O	2.41	0.40
5:F:186:LEU:HD12	5:F:186:LEU:C	2.41	0.40
3:I:23:LEU:HD23	3:I:23:LEU:HA	1.91	0.40
4:C:116:VAL:O	4:C:205:LYS:HE3	2.19	0.40
1:L:61:ARG:NH1	1:L:76:SER:O	2.54	0.40
2:B:50:LEU:HG	2:B:59:ALA:HB3	2.03	0.40
2:B:132:LEU:HB2	2:B:147:GLY:O	2.21	0.40
5:F:194:SER:HA	5:F:197:LEU:HD21	2.03	0.40
1:L:34:HIS:O	1:L:88:CYS:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:151:LYS:O	2:H:185:SER:HB2	2.21	0.40
3:G:89:ASP:HB3	3:G:92:MET:HB2	2.04	0.40
4:E:187:LYS:HB3	4:E:187:LYS:HE3	1.96	0.40
2:B:209:LYS:HB2	2:B:210:PRO:HD3	2.03	0.40
4:C:7:GLN:HB3	4:C:102:THR:OG1	2.22	0.40
4:C:204:GLU:HG2	4:C:205:LYS:N	2.36	0.40
4:E:23:CYS:O	4:E:70:THR:HA	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:317:HOH:O	7:E:322:HOH:O[4_555]	2.13	0.07

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	206/215 (96%)	196 (95%)	10 (5%)	0	100	100
1	L	206/215 (96%)	200 (97%)	6 (3%)	0	100	100
2	B	208/224 (93%)	203 (98%)	5 (2%)	0	100	100
2	H	215/224 (96%)	207 (96%)	8 (4%)	0	100	100
3	G	92/122 (75%)	90 (98%)	2 (2%)	0	100	100
3	I	91/122 (75%)	88 (97%)	3 (3%)	0	100	100
4	C	204/212 (96%)	194 (95%)	9 (4%)	1 (0%)	25	46
4	E	210/212 (99%)	202 (96%)	8 (4%)	0	100	100
5	D	197/224 (88%)	189 (96%)	8 (4%)	0	100	100
5	F	213/224 (95%)	201 (94%)	12 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1842/1994 (92%)	1770 (96%)	71 (4%)	1 (0%)	48 71

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	C	55	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	182/187 (97%)	175 (96%)	7 (4%)	28 53
1	L	182/187 (97%)	175 (96%)	7 (4%)	28 53
2	B	184/192 (96%)	177 (96%)	7 (4%)	28 53
2	H	189/192 (98%)	169 (89%)	20 (11%)	5 12
3	G	92/115 (80%)	86 (94%)	6 (6%)	14 31
3	I	92/115 (80%)	88 (96%)	4 (4%)	25 49
4	C	176/181 (97%)	166 (94%)	10 (6%)	17 37
4	E	181/181 (100%)	172 (95%)	9 (5%)	20 42
5	D	171/187 (91%)	159 (93%)	12 (7%)	12 28
5	F	181/187 (97%)	172 (95%)	9 (5%)	20 42
All	All	1630/1724 (94%)	1539 (94%)	91 (6%)	17 37

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	63	SER
1	L	107	THR
1	L	144	ARG
1	L	165	VAL
1	L	171	LYS
1	L	185	LYS

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Mol	Chain	Res	Type
1	L	201	GLN
2	H	28	ARG
2	H	57	ASP
2	H	62	GLN
2	H	74	THR
2	H	91	THR
2	H	93	VAL
2	H	117	VAL
2	H	119	VAL
2	H	124	THR
2	H	158	VAL
2	H	159	THR
2	H	169	SER
2	H	177	VAL
2	H	180	SER
2	H	194	SER
2	H	199	THR
2	H	201	THR
2	H	204	CYS
2	H	214	LYS
2	H	218	LYS
2	B	78	THR
2	B	98	ARG
2	B	117	VAL
2	B	161	SER
2	B	168	THR
2	B	169	SER
2	B	197	LEU
3	G	50	ARG
3	G	68	THR
3	G	88	GLN
3	G	90	ARG
3	G	94	GLN
3	G	98	ARG
3	I	50	ARG
3	I	80	MET
3	I	90	ARG
3	I	98	ARG
4	C	13	VAL
4	C	18	THR
4	C	53	GLN
4	C	54	ARG

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Mol	Chain	Res	Type
4	C	55	PRO
4	C	56	SER
4	C	74	THR
4	C	157	LYS
4	C	180	SER
4	C	187	LYS
5	D	17	SER
5	D	91	THR
5	D	124	THR
5	D	146	LEU
5	D	163	ASN
5	D	177	VAL
5	D	180	SER
5	D	192	VAL
5	D	201	THR
5	D	204	CYS
5	D	205	ASN
5	D	218	LYS
4	E	18	THR
4	E	27	LYS
4	E	56	SER
4	E	74	THR
4	E	105	THR
4	E	115	THR
4	E	157	LYS
4	E	176	SER
4	E	188	SER
5	F	11	LEU
5	F	17	SER
5	F	62	ASP
5	F	68	LEU
5	F	100	LYS
5	F	124	THR
5	F	173	THR
5	F	195	SER
5	F	205	ASN
1	A	54	ARG
1	A	107	THR
1	A	124	ASP
1	A	147	LYS
1	A	152	VAL
1	A	184	SER

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Mol	Chain	Res	Type
1	A	213	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	154	ASN
1	L	162	GLN
2	H	1	GLN
2	H	207	ASN
2	B	172	HIS
3	I	94	GLN
3	I	108	ASN
4	C	42	GLN
5	D	207	ASN
4	E	38	GLN
4	E	109	GLN
5	F	39	GLN
5	F	113	GLN
5	F	179	GLN
1	A	149	GLN
1	A	157	GLN
1	A	160	ASN

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

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	ACT	A	301	-	3,3,3	1.46	0	3,3,3	1.59	1 (33%)
6	ACT	L	301	-	3,3,3	1.93	2 (66%)	3,3,3	1.54	1 (33%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	301	ACT	CH3-C	2.54	1.59	1.49
6	L	301	ACT	O-C	2.06	1.31	1.22

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	301	ACT	OXT-C-O	2.18	130.10	122.03
6	L	301	ACT	OXT-C-O	2.03	129.56	122.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	301	ACT	1	0
6	L	301	ACT	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	210/215 (97%)	0.16	8 (3%) 44 43	50, 88, 140, 166	0
1	L	210/215 (97%)	-0.23	2 (0%) 79 78	54, 80, 112, 146	0
2	B	214/224 (95%)	-0.12	6 (2%) 55 53	43, 72, 131, 155	0
2	H	219/224 (97%)	-0.42	2 (0%) 81 80	44, 60, 116, 133	0
3	G	96/122 (78%)	-0.14	0 100 100	53, 77, 125, 179	0
3	I	95/122 (77%)	-0.17	0 100 100	55, 78, 117, 176	0
4	C	206/212 (97%)	-0.18	6 (2%) 54 52	48, 77, 131, 149	0
4	E	212/212 (100%)	-0.43	0 100 100	45, 67, 105, 131	0
5	D	206/224 (91%)	-0.01	8 (3%) 44 42	51, 81, 130, 151	0
5	F	217/224 (96%)	0.07	4 (1%) 67 67	50, 89, 133, 150	0
All	All	1885/1994 (94%)	-0.15	36 (1%) 66 65	43, 77, 129, 179	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	C	52	ASN	6.1
5	D	194	SER	4.8
5	D	142	GLY	4.3
2	B	199	THR	3.9
1	A	58	ILE	3.6
4	C	119	PHE	3.4
5	D	132	LEU	3.1
2	B	174	PHE	3.1
1	L	58	ILE	3.0
5	F	157	PRO	3.0
1	L	49	SER	2.9
1	A	152	VAL	2.9
1	A	124	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	198	GLY	2.8
2	H	140	SER	2.7
2	B	136	SER	2.7
4	C	51	THR	2.6
1	A	155	ALA	2.6
5	D	144	ALA	2.6
1	A	196	CYS	2.5
4	C	53	GLN	2.5
4	C	130	LYS	2.5
1	A	59	PRO	2.3
2	H	221	PRO	2.3
5	D	193	PRO	2.3
2	B	135	SER	2.3
5	D	170	GLY	2.3
5	F	43	LYS	2.2
1	A	183	LEU	2.2
2	B	134	PRO	2.2
5	D	133	ALA	2.2
5	D	169	SER	2.2
1	A	214	GLY	2.2
5	F	135	SER	2.0
4	C	55	PRO	2.0
5	F	188	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	ACT	A	301	4/4	0.56	0.29	70,77,88,88	0
6	ACT	L	301	4/4	0.72	0.20	73,77,92,92	0

6.5 Other polymers (i)

There are no such residues in this entry.