Full wwPDB X-ray Structure Validation Report ⓘ

Jul 4, 2024 – 12:22 PM JST

PDB ID	:	8XK8
Title	:	N1D10 Fab bound to SFTSV glycoprotein-Gn
Authors	:	Zhao, H.; Deng, Z.
Deposited on	:	2023-12-22
Resolution	:	3.53 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:

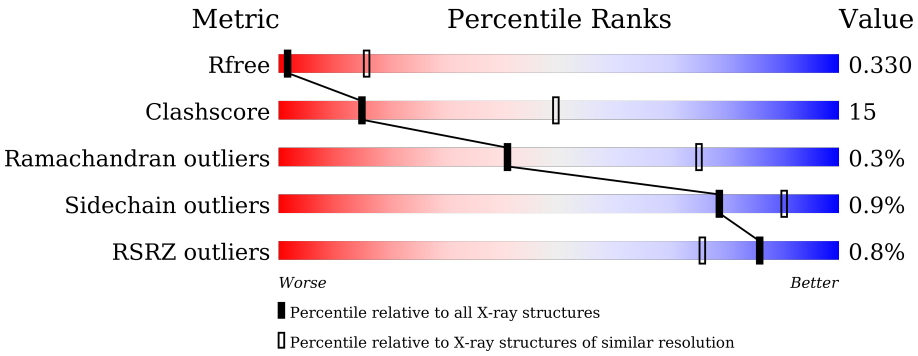
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.53 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	1028 (3.60-3.48)
Clashscore	141614	1109 (3.60-3.48)
Ramachandran outliers	138981	1073 (3.60-3.48)
Sidechain outliers	138945	1074 (3.60-3.48)
RSRZ outliers	127900	1079 (3.62-3.46)

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	357	51% 36% · 12%
1	B	357	2% 62% 25% 12%
2	C	247	% 64% 23% · 13%
2	H	247	62% 25% · 13%
3	D	238	67% 25% 8%
3	L	238	58% 33% · 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11394 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 Envelopment polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	0	0
			2398	1503	415	454	26			
1	B	313	Total	C	N	O	S	0	0	0
			2402	1506	416	454	26			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	LEU	PHE	conflict	UNP R4V2Q5
A	18	GLY	SER	conflict	UNP R4V2Q5
A	21	THR	SER	conflict	UNP R4V2Q5
A	161	ARG	GLY	conflict	UNP R4V2Q5
A	340	SER	-	expression tag	UNP R4V2Q5
A	341	GLY	-	expression tag	UNP R4V2Q5
A	342	SER	-	expression tag	UNP R4V2Q5
A	343	THR	-	expression tag	UNP R4V2Q5
A	344	LEU	-	expression tag	UNP R4V2Q5
A	345	GLU	-	expression tag	UNP R4V2Q5
A	346	VAL	-	expression tag	UNP R4V2Q5
A	347	LEU	-	expression tag	UNP R4V2Q5
A	348	PHE	-	expression tag	UNP R4V2Q5
A	349	GLN	-	expression tag	UNP R4V2Q5
A	350	GLY	-	expression tag	UNP R4V2Q5
A	351	PRO	-	expression tag	UNP R4V2Q5
A	352	HIS	-	expression tag	UNP R4V2Q5
A	353	HIS	-	expression tag	UNP R4V2Q5
A	354	HIS	-	expression tag	UNP R4V2Q5
A	355	HIS	-	expression tag	UNP R4V2Q5
A	356	HIS	-	expression tag	UNP R4V2Q5
A	357	HIS	-	expression tag	UNP R4V2Q5
B	13	LEU	PHE	conflict	UNP R4V2Q5
B	18	GLY	SER	conflict	UNP R4V2Q5
B	21	THR	SER	conflict	UNP R4V2Q5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	161	ARG	GLY	conflict	UNP R4V2Q5
B	340	SER	-	expression tag	UNP R4V2Q5
B	341	GLY	-	expression tag	UNP R4V2Q5
B	342	SER	-	expression tag	UNP R4V2Q5
B	343	THR	-	expression tag	UNP R4V2Q5
B	344	LEU	-	expression tag	UNP R4V2Q5
B	345	GLU	-	expression tag	UNP R4V2Q5
B	346	VAL	-	expression tag	UNP R4V2Q5
B	347	LEU	-	expression tag	UNP R4V2Q5
B	348	PHE	-	expression tag	UNP R4V2Q5
B	349	GLN	-	expression tag	UNP R4V2Q5
B	350	GLY	-	expression tag	UNP R4V2Q5
B	351	PRO	-	expression tag	UNP R4V2Q5
B	352	HIS	-	expression tag	UNP R4V2Q5
B	353	HIS	-	expression tag	UNP R4V2Q5
B	354	HIS	-	expression tag	UNP R4V2Q5
B	355	HIS	-	expression tag	UNP R4V2Q5
B	356	HIS	-	expression tag	UNP R4V2Q5
B	357	HIS	-	expression tag	UNP R4V2Q5

- Molecule 2 is a protein called mAb N1D10 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	216	Total	C	N	O	S	0	0	0
			1608	1014	265	322	7			
2	C	216	Total	C	N	O	S	0	0	0
			1608	1014	265	322	7			

- Molecule 3 is a protein called mAb N1D10 Fab light chain.

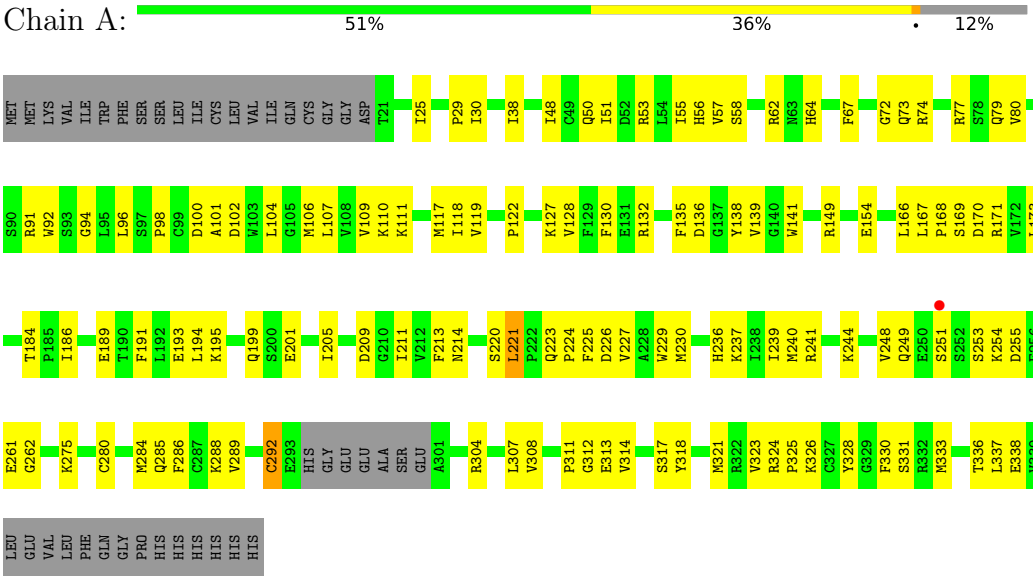
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	219	Total	C	N	O	S	0	0	0
			1689	1064	282	336	7			
3	D	219	Total	C	N	O	S	0	0	0
			1689	1064	282	336	7			

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: Envelopment polyprotein

Chain A:

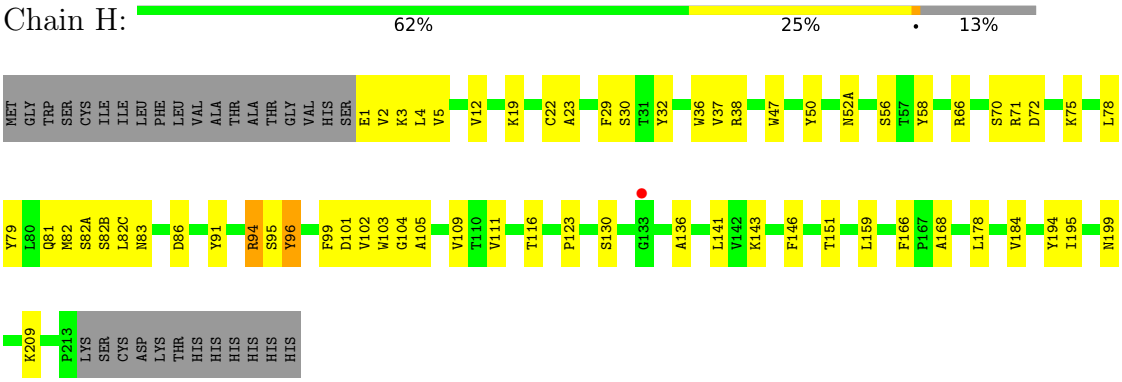


• Molecule 1: Envelopment polyprotein

Chain B:

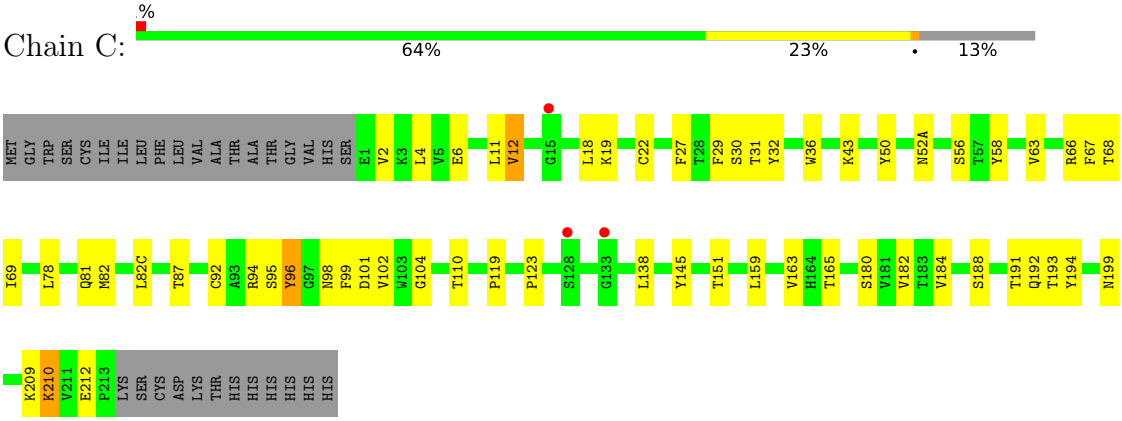
• Molecule 2: mAb N1D10 Fab heavy chain

Chain H:



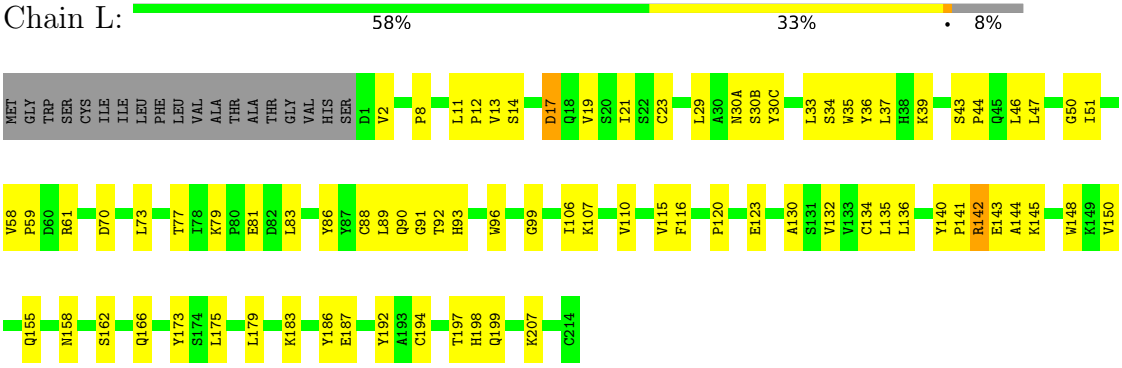
• Molecule 2: mAb N1D10 Fab heavy chain

Chain C:



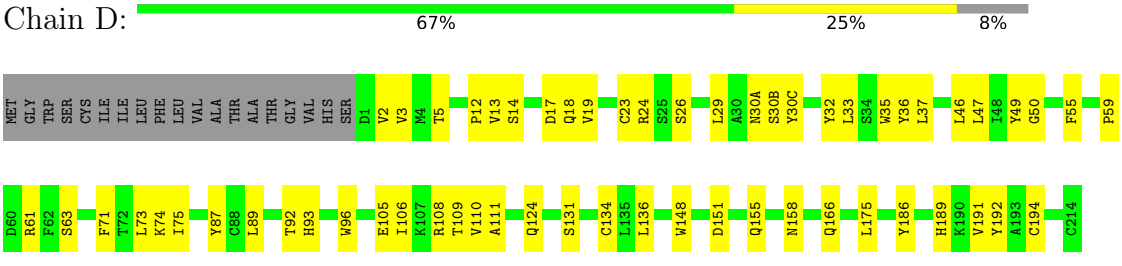
• Molecule 3: mAb N1D10 Fab light chain

Chain L:



• Molecule 3: mAb N1D10 Fab light chain

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	84.12Å 111.91Å 87.86Å 90.00° 94.33° 90.00°	Depositor
Resolution (Å)	20.69 – 3.53 47.16 – 3.53	Depositor EDS
% Data completeness (in resolution range)	99.0 (20.69-3.53) 87.7 (47.16-3.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.46 (at 3.57Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.250 , 0.324 0.255 , 0.330	Depositor DCC
R_{free} test set	1089 reflections (5.48%)	wwPDB-VP
Wilson B-factor (Å^2)	-5.0	Xtriage
Anisotropy	-19.391	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , -24.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.055 for l,-k,h	Xtriage
F_o,F_c correlation	0.81	EDS
Total number of atoms	11394	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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

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	0.30	0/2458	0.54	0/3317
1	B	0.31	0/2462	0.55	0/3321
2	C	0.31	0/1647	0.59	1/2245 (0.0%)
2	H	0.31	0/1647	0.57	0/2245
3	D	0.32	0/1729	0.54	0/2346
3	L	0.35	0/1729	0.55	0/2346
All	All	0.32	0/11672	0.56	1/15820 (0.0%)

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
2	C	0	1
2	H	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	210	LYS	CD-CE-NZ	5.16	123.57	111.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	95	SER	Peptide
2	H	94	ARG	Peptide

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	2398	0	2296	113	0
1	B	2402	0	2307	69	0
2	C	1608	0	1571	41	0
2	H	1608	0	1571	53	0
3	D	1689	0	1645	38	1
3	L	1689	0	1645	64	1
All	All	11394	0	11035	340	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 15.

All (340) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:TYR:OH	2:C:56:SER:OG	2.02	0.78
1:B:201:GLU:O	1:B:241:ARG:NH2	2.17	0.77
2:H:66:ARG:NH1	2:H:82(B):SER:O	2.19	0.75
3:D:108:ARG:HH21	3:D:111:ALA:HB2	1.52	0.73
3:D:13:VAL:HG12	3:D:19:VAL:HG11	1.71	0.72
2:C:22:CYS:HB3	2:C:78:LEU:HB3	1.72	0.71
1:A:72:GLY:HA2	1:A:169:SER:HB3	1.72	0.71
3:L:106:ILE:O	3:L:166:GLN:NE2	2.24	0.70
1:A:83:TYR:OH	2:H:56:SER:OG	2.10	0.69
1:A:135:PHE:HD2	1:A:211:ILE:HB	1.57	0.69
1:A:201:GLU:O	1:A:241:ARG:NH2	2.26	0.69
2:H:22:CYS:HB3	2:H:78:LEU:HB3	1.78	0.66
1:B:207:LYS:HE2	1:B:219:GLU:OE1	1.95	0.66
2:H:50:TYR:HD2	2:H:58:TYR:HD2	1.44	0.65
1:A:64:HIS:HB3	1:A:111:LYS:HD3	1.78	0.65
1:B:221:LEU:HD13	3:D:32:TYR:HA	1.78	0.65
2:C:159:LEU:HD21	2:C:182:VAL:HG21	1.79	0.65
1:A:201:GLU:OE1	1:A:318:TYR:OH	2.07	0.65
3:L:136:LEU:HD22	3:L:175:LEU:HD22	1.78	0.65
3:L:47:LEU:HA	3:L:58:VAL:HG21	1.80	0.64
1:B:61:LEU:HD21	1:B:129:PHE:HB2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:VAL:O	1:A:312:GLY:HA3	1.98	0.64
1:B:72:GLY:HA2	1:B:169:SER:OG	1.98	0.64
1:A:25:ILE:HA	1:B:288:LYS:NZ	2.13	0.64
2:H:5:VAL:HG23	2:H:23:ALA:HB3	1.81	0.63
2:C:123:PRO:HD3	2:C:209:LYS:HE2	1.80	0.63
1:A:338:GLU:HG2	1:A:340:SER:H	1.64	0.62
3:L:83:LEU:HD11	3:L:106:ILE:HD11	1.82	0.61
2:H:50:TYR:CD2	2:H:58:TYR:HD2	2.19	0.61
1:A:117:MET:HA	3:L:30(C):TYR:CZ	2.36	0.61
1:A:244:LYS:HB2	1:A:317:SER:HB3	1.81	0.61
1:B:125:LYS:HD3	1:B:151:GLU:HB3	1.83	0.60
3:L:12:PRO:HB3	3:L:140:TYR:OH	2.01	0.60
3:D:108:ARG:HG3	3:D:109:THR:H	1.67	0.60
3:D:136:LEU:HB2	3:D:175:LEU:HB3	1.83	0.59
3:L:144:ALA:HB2	3:L:198:HIS:HD2	1.68	0.59
1:A:119:VAL:HG22	1:A:132:ARG:HD2	1.84	0.59
2:H:82:MET:HB3	2:H:82(C):LEU:HD21	1.85	0.58
1:A:230:MET:HG3	1:A:325:PRO:HB3	1.85	0.58
2:H:130:SER:HA	3:L:116:PHE:HD1	1.68	0.58
1:A:79:GLN:HB2	1:A:169:SER:OG	2.03	0.58
2:H:209:LYS:NZ	3:L:123:GLU:OE1	2.23	0.58
1:A:226:ASP:O	2:H:52(A):ASN:ND2	2.37	0.58
2:H:94:ARG:O	2:H:99:PHE:HA	2.04	0.58
1:A:227:VAL:HG21	1:A:239:ILE:HB	1.86	0.58
1:B:232:VAL:HG12	1:B:323:VAL:HG11	1.86	0.58
1:B:89:TYR:HH	1:B:328:TYR:HE2	1.51	0.57
1:A:101:ALA:HB1	1:A:106:MET:HB2	1.86	0.57
2:C:11:LEU:HD23	2:C:18:LEU:HD12	1.85	0.57
1:A:184:THR:HG23	1:A:324:ARG:HD2	1.85	0.57
1:B:229:TRP:HE1	1:B:331:SER:HB3	1.68	0.56
1:A:205:ILE:O	1:A:214:ASN:HB2	2.06	0.56
1:B:48:ILE:HD13	1:B:51:ILE:HD12	1.87	0.56
1:B:229:TRP:HE1	1:B:331:SER:CB	2.19	0.56
2:H:71:ARG:HB3	2:H:78:LEU:HD12	1.86	0.56
3:L:36:TYR:HE2	3:L:89:LEU:HB3	1.71	0.56
3:L:39:LYS:NZ	3:L:81:GLU:HA	2.20	0.56
1:A:132:ARG:HH22	1:A:209:ASP:CG	2.10	0.55
1:B:56:HIS:NE2	1:B:100:ASP:OD1	2.39	0.55
1:A:285:GLN:OE1	1:A:307:LEU:HD22	2.06	0.55
1:B:205:ILE:O	1:B:214:ASN:HB2	2.06	0.55
3:L:21:ILE:HD12	3:L:73:LEU:HD23	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:PRO:HG2	1:A:171:ARG:HG2	1.89	0.55
2:H:38:ARG:NH1	2:H:86:ASP:OD1	2.31	0.55
3:L:33:LEU:HD23	3:L:34:SER:N	2.22	0.55
1:A:73:GLN:HG3	1:A:166:LEU:HB3	1.90	0.54
1:A:48:ILE:HD11	1:A:104:LEU:HD11	1.89	0.54
1:A:122:PRO:HB3	1:A:173:LEU:HD21	1.89	0.54
2:C:11:LEU:HB3	2:C:18:LEU:HD13	1.90	0.54
1:B:154:GLU:HG2	3:D:30(B):SER:HB2	1.90	0.53
3:L:35:TRP:CD2	3:L:73:LEU:HB2	2.42	0.53
3:L:107:LYS:HA	3:L:140:TYR:OH	2.09	0.53
2:C:2:VAL:HG11	2:C:102:VAL:HG21	1.89	0.53
1:A:107:LEU:HD13	1:A:138:TYR:CD1	2.44	0.53
1:B:261:GLU:OE2	1:B:281:ARG:NH1	2.36	0.53
1:A:261:GLU:OE2	1:A:304:ARG:HD3	2.08	0.53
2:H:32:TYR:CD2	2:H:94:ARG:HD2	2.43	0.53
3:L:61:ARG:HD2	3:L:77:THR:O	2.09	0.52
2:C:210:LYS:HE2	2:C:212:GLU:HG3	1.91	0.52
2:C:119:PRO:HB3	2:C:145:TYR:HB3	1.91	0.52
3:L:14:SER:O	3:L:17:ASP:HB2	2.09	0.52
1:A:257:VAL:HG13	1:A:308:VAL:HG22	1.91	0.52
1:B:118:ILE:HG13	3:D:30(C):TYR:OH	2.10	0.52
3:D:3:VAL:HB	3:D:26:SER:HB3	1.91	0.52
1:A:191:PHE:HA	1:A:194:LEU:HD12	1.90	0.52
2:H:103:TRP:CD2	3:L:44:PRO:HB2	2.45	0.52
2:C:2:VAL:HG12	2:C:102:VAL:HG11	1.92	0.52
2:H:12:VAL:HG11	2:H:82(C):LEU:HD13	1.91	0.51
3:D:59:PRO:HB2	3:D:61:ARG:HG2	1.92	0.51
1:B:226:ASP:HB3	1:B:330:PHE:CE1	2.45	0.51
3:L:88:CYS:O	3:L:99:GLY:N	2.43	0.51
2:H:2:VAL:HG11	2:H:102:VAL:HG21	1.91	0.51
1:A:248:VAL:HG22	1:A:313:GLU:HB2	1.93	0.51
1:A:314:VAL:O	1:A:325:PRO:HD2	2.11	0.51
1:A:314:VAL:HG21	1:A:328:TYR:CD2	2.46	0.51
3:D:155:GLN:OE1	3:D:158:ASN:ND2	2.43	0.51
1:B:49:CYS:SG	1:B:53:ARG:NH1	2.83	0.51
1:B:218:GLY:O	1:B:339:VAL:N	2.44	0.51
1:B:260:LYS:HD3	1:B:302:LYS:O	2.11	0.51
1:A:62:ARG:HG2	1:A:67:PHE:O	2.12	0.50
1:A:229:TRP:HE1	1:A:331:SER:CB	2.24	0.50
2:C:188:SER:O	2:C:192:GLN:N	2.39	0.50
2:H:116:THR:HA	2:H:146:PHE:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:29:PHE:O	2:H:71:ARG:NH2	2.42	0.50
1:A:30:ILE:HG23	1:A:74:ARG:HE	1.76	0.50
1:B:241:ARG:HH12	2:C:31:THR:CG2	2.24	0.50
1:B:119:VAL:HB	1:B:332:ARG:HG2	1.94	0.50
1:B:147:LYS:HB3	1:B:156:CYS:HB3	1.93	0.50
3:L:37:LEU:HB2	3:L:47:LEU:HD11	1.94	0.49
3:L:186:TYR:HA	3:L:192:TYR:OH	2.12	0.49
1:B:184:THR:HG23	1:B:324:ARG:HD2	1.94	0.49
1:A:128:VAL:HG21	1:A:167:LEU:HD13	1.92	0.49
2:H:96:TYR:HA	3:L:96:TRP:CH2	2.47	0.49
3:D:23:CYS:HB2	3:D:35:TRP:CH2	2.48	0.49
1:B:220:SER:HB2	2:C:98:ASN:ND2	2.28	0.49
1:A:92:TRP:CD2	1:A:311:PRO:HD3	2.48	0.49
1:A:106:MET:O	1:A:326:LYS:HD2	2.13	0.49
1:A:304:ARG:HH22	1:B:284:MET:HE3	1.78	0.49
2:C:165:THR:HA	2:C:180:SER:HA	1.94	0.49
1:A:205:ILE:HA	1:A:337:LEU:HD22	1.95	0.49
2:C:12:VAL:HG11	2:C:82(C):LEU:HD13	1.94	0.49
2:C:138:LEU:HD21	2:C:194:TYR:CD2	2.48	0.49
1:A:261:GLU:OE1	1:B:287:CYS:HB3	2.12	0.49
1:A:284:MET:HG2	1:A:288:LYS:HD3	1.95	0.49
1:B:228:ALA:O	1:B:240:MET:N	2.41	0.49
2:H:72:ASP:OD2	2:H:75:LYS:HE3	2.13	0.49
3:L:120:PRO:HG3	3:L:130:ALA:HB1	1.93	0.49
1:B:202:PHE:CE1	1:B:239:ILE:HG13	2.48	0.48
1:A:132:ARG:HG2	1:A:141:TRP:CZ3	2.48	0.48
1:B:37:ASP:HA	1:B:62:ARG:HH12	1.78	0.48
2:C:30:SER:O	2:C:52(A):ASN:HB2	2.13	0.48
3:L:29:LEU:HD12	3:L:33:LEU:HD12	1.95	0.48
1:A:154:GLU:HG2	3:L:30(B):SER:HB2	1.96	0.48
3:L:59:PRO:HB2	3:L:61:ARG:HG2	1.94	0.48
1:B:80:VAL:HG21	1:B:174:TRP:CE3	2.49	0.48
1:B:207:LYS:HG2	1:B:212:VAL:HA	1.95	0.48
1:A:130:PHE:HE2	1:A:149:ARG:HD2	1.79	0.48
1:B:269:SER:HA	1:B:272:LYS:HE2	1.95	0.48
1:B:83:TYR:CG	1:B:122:PRO:HG3	2.49	0.48
2:C:2:VAL:HG13	2:C:27:PHE:CD1	2.49	0.48
1:A:253:SER:HB3	1:A:275:LYS:HD2	1.95	0.47
2:C:50:TYR:CD2	2:C:58:TYR:HD2	2.32	0.47
1:A:127:LYS:HE2	1:A:173:LEU:HB2	1.97	0.47
3:D:106:ILE:O	3:D:166:GLN:NE2	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:50:GLY:O	3:L:51:ILE:HB	2.13	0.47
1:A:77:ARG:O	1:A:80:VAL:HG22	2.15	0.47
1:A:240:MET:HG2	1:A:318:TYR:CZ	2.49	0.47
1:A:255:ASP:O	1:A:308:VAL:HG23	2.14	0.47
2:H:30:SER:O	2:H:52(A):ASN:HB2	2.14	0.47
1:B:231:ASP:O	1:B:326:LYS:N	2.46	0.47
2:H:123:PRO:HD3	2:H:209:LYS:HE2	1.95	0.47
2:H:184:VAL:HG11	2:H:194:TYR:CE1	2.50	0.47
1:A:29:PRO:HD3	1:A:53:ARG:HA	1.97	0.47
1:A:260:LYS:HB2	1:A:260:LYS:HE2	1.67	0.47
1:B:183:MET:SD	1:B:233:GLY:HA3	2.55	0.47
1:B:256:PHE:O	1:B:275:LYS:NZ	2.33	0.47
2:C:63:VAL:HG12	2:C:66:ARG:NH2	2.30	0.47
1:A:229:TRP:CZ3	1:A:237:LYS:HE2	2.50	0.47
1:A:259:TYR:CE2	1:B:288:LYS:HE2	2.50	0.47
1:B:204:ASP:OD1	1:B:204:ASP:N	2.43	0.47
3:L:61:ARG:CZ	3:L:79:LYS:HG3	2.45	0.47
3:L:35:TRP:CZ3	3:L:88:CYS:HB3	2.50	0.47
3:L:37:LEU:HD13	3:L:86:TYR:CZ	2.50	0.47
3:L:110:VAL:HG21	3:L:199:GLN:NE2	2.30	0.47
1:B:31:HIS:HB2	1:B:166:LEU:HD22	1.97	0.46
2:C:184:VAL:HG11	2:C:194:TYR:CE1	2.50	0.46
1:A:135:PHE:CD2	1:A:211:ILE:HB	2.45	0.46
1:B:127:LYS:HE2	1:B:173:LEU:HB2	1.97	0.46
3:D:29:LEU:HD12	3:D:71:PHE:CE1	2.50	0.46
1:A:280:CYS:O	1:A:292:CYS:HA	2.14	0.46
1:B:241:ARG:HH12	2:C:31:THR:HG23	1.80	0.46
2:H:105:ALA:HA	3:L:43:SER:HG	1.81	0.46
3:L:140:TYR:CG	3:L:141:PRO:HA	2.51	0.46
3:D:151:ASP:HA	3:D:191:VAL:HB	1.97	0.46
1:A:136:ASP:HB3	1:A:211:ILE:HG13	1.96	0.46
1:A:285:GLN:O	1:A:289:VAL:HG22	2.15	0.46
3:L:11:LEU:O	3:L:13:VAL:HG13	2.15	0.46
1:A:88:SER:HA	1:A:91:ARG:HH11	1.79	0.46
1:B:56:HIS:HB3	1:B:103:TRP:CG	2.50	0.46
1:B:120:PRO:CG	1:B:224:PRO:HG3	2.46	0.46
3:L:145:LYS:HB3	3:L:197:THR:HB	1.96	0.46
2:C:27:PHE:CE2	2:C:29:PHE:HA	2.51	0.46
1:A:106:MET:HE1	1:A:181:GLN:N	2.30	0.46
3:D:18:GLN:HA	3:D:75:ILE:O	2.15	0.46
3:D:134:CYS:HB2	3:D:148:TRP:CH2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ILE:HA	1:B:288:LYS:HZ3	1.78	0.46
1:A:102:ASP:HA	1:A:107:LEU:O	2.16	0.46
2:C:36:TRP:HD1	2:C:69:ILE:HD12	1.81	0.46
1:B:122:PRO:HB3	1:B:173:LEU:HD21	1.98	0.46
3:L:142:ARG:HH11	3:L:143:GLU:HG3	1.81	0.46
1:A:92:TRP:CG	1:A:311:PRO:HD3	2.50	0.45
1:A:94:GLY:HA3	1:A:308:VAL:HG12	1.98	0.45
1:A:255:ASP:O	1:A:307:LEU:HD12	2.17	0.45
2:H:83:ASN:OD1	2:H:83:ASN:N	2.47	0.45
1:A:58:SER:O	1:A:62:ARG:HG3	2.16	0.45
2:C:151:THR:OG1	2:C:199:ASN:HB3	2.15	0.45
1:B:77:ARG:NE	1:B:100:ASP:OD2	2.47	0.45
2:H:52(A):ASN:OD1	2:H:52(A):ASN:N	2.44	0.45
3:L:91:GLY:HA2	3:L:96:TRP:CD1	2.51	0.45
3:D:37:LEU:HB2	3:D:47:LEU:HD11	1.97	0.45
1:A:223:GLN:NE2	2:H:95:SER:O	2.49	0.45
1:A:79:GLN:OE1	1:B:248:VAL:HG12	2.17	0.45
1:B:229:TRP:CE3	1:B:237:LYS:HD3	2.51	0.45
3:D:5:THR:O	3:D:23:CYS:HA	2.17	0.45
1:A:83:TYR:CG	1:A:122:PRO:HG3	2.52	0.45
3:L:132:VAL:HB	3:L:179:LEU:HB3	1.97	0.45
1:A:128:VAL:HG23	1:A:171:ARG:HB3	1.98	0.45
1:A:337:LEU:HD12	2:H:32:TYR:CE2	2.51	0.45
1:B:101:ALA:HB1	1:B:106:MET:HB2	1.99	0.45
2:H:168:ALA:HA	2:H:178:LEU:HB3	1.98	0.45
1:A:136:ASP:OD2	1:A:211:ILE:HD11	2.17	0.45
2:C:87:THR:HG23	2:C:110:THR:HA	1.97	0.45
3:D:186:TYR:HA	3:D:192:TYR:OH	2.16	0.45
1:A:132:ARG:NH2	1:A:209:ASP:OD2	2.50	0.45
1:B:339:VAL:HG21	3:D:49:TYR:CZ	2.52	0.45
2:H:105:ALA:HA	3:L:43:SER:OG	2.16	0.45
1:A:50:GLN:HB3	1:A:55:ILE:HB	1.99	0.44
3:L:89:LEU:HG	3:L:90:GLN:O	2.17	0.44
3:D:30(A):ASN:HB3	3:D:92:THR:HG23	1.99	0.44
3:D:148:TRP:HB2	3:D:155:GLN:HB2	1.99	0.44
1:A:186:ILE:HG21	1:A:323:VAL:HG12	1.99	0.44
2:H:52(A):ASN:HA	2:H:71:ARG:NH1	2.33	0.44
3:L:8:PRO:HG2	3:L:11:LEU:HB2	1.99	0.44
3:L:115:VAL:HA	3:L:135:LEU:O	2.17	0.44
3:D:124:GLN:HE22	3:D:131:SER:CB	2.30	0.44
1:A:38:ILE:HG23	1:A:62:ARG:NH1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:GLU:HG2	1:A:241:ARG:NH2	2.32	0.44
2:H:75:LYS:HE2	2:H:75:LYS:HB3	1.87	0.44
3:L:13:VAL:CG1	3:L:19:VAL:HG11	2.48	0.44
3:D:12:PRO:HA	3:D:105:GLU:O	2.18	0.44
2:C:99:PHE:N	3:D:36:TYR:OH	2.42	0.44
2:C:193:THR:HA	2:C:212:GLU:OE2	2.17	0.44
1:A:130:PHE:HA	1:A:173:LEU:O	2.18	0.43
1:A:118:ILE:N	3:L:30(C):TYR:OH	2.43	0.43
2:C:96:TYR:HA	3:D:96:TRP:CH2	2.53	0.43
1:A:336:THR:C	1:A:337:LEU:HD23	2.39	0.43
3:D:189:HIS:HB2	3:D:192:TYR:OH	2.18	0.43
1:A:226:ASP:HB3	1:A:330:PHE:CE1	2.54	0.43
1:B:128:VAL:HG21	1:B:167:LEU:HD13	2.00	0.43
2:H:37:VAL:O	2:H:91:TYR:N	2.34	0.43
2:H:99:PHE:O	2:H:103:TRP:NE1	2.51	0.43
2:H:166:PHE:HB3	3:L:162:SER:OG	2.19	0.43
2:C:101:ASP:N	2:C:101:ASP:OD1	2.50	0.43
3:L:29:LEU:HA	3:L:93:HIS:HE2	1.84	0.43
2:C:43:LYS:O	3:D:87:TYR:OH	2.21	0.43
3:D:46:LEU:HD23	3:D:55:PHE:CD1	2.54	0.43
1:A:229:TRP:HE1	1:A:331:SER:HB2	1.82	0.43
1:A:275:LYS:HG2	1:A:286:PHE:HZ	1.82	0.43
2:H:4:LEU:HD12	2:H:102:VAL:HG12	2.00	0.43
2:H:141:LEU:HD21	2:H:143:LYS:HD2	2.01	0.43
3:L:110:VAL:HG22	3:L:141:PRO:HD3	2.00	0.43
1:A:195:LYS:HE3	1:A:236:HIS:CE1	2.54	0.43
1:A:275:LYS:HG2	1:A:286:PHE:CZ	2.53	0.43
2:H:70:SER:O	2:H:79:TYR:N	2.48	0.43
3:L:158:ASN:O	3:L:179:LEU:HD12	2.19	0.43
1:A:56:HIS:CD2	1:A:57:VAL:HG23	2.54	0.43
1:A:127:LYS:HE3	1:A:170:ASP:O	2.19	0.43
1:B:120:PRO:HG2	1:B:224:PRO:HG3	2.00	0.43
2:H:47:TRP:HZ2	2:H:50:TYR:HB3	1.83	0.43
3:L:36:TYR:CE1	3:L:46:LEU:HD13	2.54	0.43
1:B:248:VAL:O	1:B:312:GLY:HA3	2.18	0.43
2:H:1:GLU:CG	2:H:3:LYS:HD2	2.48	0.43
2:H:159:LEU:HD12	2:H:159:LEU:HA	1.93	0.43
3:L:2:VAL:HB	3:L:90:GLN:NE2	2.34	0.43
1:B:219:GLU:O	1:B:219:GLU:HG2	2.18	0.42
1:B:154:GLU:HG2	3:D:30(B):SER:CB	2.47	0.42
1:B:248:VAL:HG22	1:B:313:GLU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:35:TRP:CD2	3:D:73:LEU:HB2	2.54	0.42
1:A:154:GLU:HG2	3:L:30(B):SER:CB	2.49	0.42
3:D:63:SER:OG	3:D:74:LYS:HB3	2.19	0.42
1:A:132:ARG:HH21	1:A:333:MET:HA	1.84	0.42
3:L:116:PHE:HB2	3:L:135:LEU:HB3	2.00	0.42
1:B:149:ARG:HA	1:B:155:LEU:O	2.20	0.42
2:C:94:ARG:NH2	2:C:101:ASP:OD2	2.29	0.42
3:L:148:TRP:HB2	3:L:155:GLN:HB2	2.02	0.42
1:A:96:LEU:HD22	1:A:100:ASP:HB3	2.00	0.42
1:A:117:MET:O	1:A:132:ARG:NH1	2.53	0.42
1:A:248:VAL:CG2	1:A:313:GLU:HB2	2.49	0.42
3:L:30(A):ASN:HB3	3:L:92:THR:HG22	2.01	0.42
3:L:183:LYS:HE3	3:L:187:GLU:OE1	2.19	0.42
2:C:6:GLU:OE2	2:C:104:GLY:HA3	2.19	0.42
3:D:14:SER:O	3:D:17:ASP:HB2	2.20	0.42
3:D:136:LEU:HD13	3:D:175:LEU:HD22	2.02	0.42
1:A:51:ILE:HA	1:A:56:HIS:ND1	2.35	0.42
2:H:66:ARG:O	2:H:82(A):SER:OG	2.23	0.42
1:A:89:TYR:CD2	1:A:179:ALA:HB2	2.55	0.42
1:A:102:ASP:HB2	1:A:109:VAL:HG23	2.02	0.42
1:A:195:LYS:HE3	1:A:236:HIS:NE2	2.35	0.42
1:B:226:ASP:O	2:C:52(A):ASN:ND2	2.53	0.42
1:B:256:PHE:HB2	1:B:275:LYS:HE2	2.01	0.42
2:H:101:ASP:OD1	2:H:101:ASP:N	2.43	0.42
1:A:221:LEU:HD11	3:L:50:GLY:CA	2.49	0.41
1:A:224:PRO:HD3	2:H:96:TYR:CE2	2.55	0.41
1:A:262:GLY:HA2	1:B:289:VAL:C	2.41	0.41
1:A:307:LEU:HD12	1:A:307:LEU:HA	1.93	0.41
1:A:314:VAL:HG11	1:A:328:TYR:HB3	2.02	0.41
3:D:151:ASP:N	3:D:191:VAL:O	2.29	0.41
3:D:36:TYR:HE1	3:D:89:LEU:HB3	1.85	0.41
1:A:199:GLN:HG2	1:A:213:PHE:O	2.20	0.41
1:B:130:PHE:HE1	1:B:149:ARG:HD2	1.85	0.41
2:H:4:LEU:O	2:H:104:GLY:HA2	2.19	0.41
3:L:158:ASN:HB3	3:L:179:LEU:HD12	2.03	0.41
3:L:173:TYR:CD1	3:L:173:TYR:N	2.88	0.41
1:A:98:PRO:HA	1:A:107:LEU:HD21	2.02	0.41
1:A:135:PHE:CZ	1:A:213:PHE:HD2	2.39	0.41
1:B:102:ASP:HA	1:B:107:LEU:O	2.20	0.41
2:H:36:TRP:HE1	2:H:78:LEU:HG	1.85	0.41
2:H:130:SER:O	2:H:136:ALA:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:GLU:O	1:A:193:GLU:HB2	2.19	0.41
1:A:225:PHE:CZ	1:A:227:VAL:HB	2.55	0.41
1:A:229:TRP:HE1	1:A:331:SER:HB3	1.86	0.41
1:A:77:ARG:C	1:A:79:GLN:H	2.23	0.41
2:H:195:ILE:HA	2:H:209:LYS:O	2.21	0.41
1:A:220:SER:O	1:A:336:THR:HB	2.20	0.41
1:B:54:LEU:HD23	1:B:56:HIS:HE1	1.85	0.41
2:H:82:MET:HE1	2:H:109:VAL:HG11	2.03	0.41
3:L:140:TYR:CD2	3:L:141:PRO:HA	2.55	0.41
3:L:140:TYR:CD2	3:L:173:TYR:HE1	2.39	0.41
3:L:207:LYS:HA	3:L:207:LYS:HD2	1.78	0.41
2:C:4:LEU:HB3	2:C:92:CYS:SG	2.61	0.41
2:C:163:VAL:HG22	2:C:182:VAL:HB	2.03	0.41
2:C:188:SER:HA	2:C:191:THR:OG1	2.20	0.41
3:D:33:LEU:O	3:D:50:GLY:N	2.53	0.41
1:A:110:LYS:O	1:A:139:VAL:HA	2.21	0.40
1:A:244:LYS:HD2	1:A:244:LYS:N	2.36	0.40
2:H:12:VAL:CG1	2:H:111:VAL:HG22	2.52	0.40
3:L:8:PRO:HG3	3:L:11:LEU:HD13	2.02	0.40
3:L:150:VAL:HG22	3:L:192:TYR:CD2	2.56	0.40
3:D:2:VAL:HG21	3:D:93:HIS:HB2	2.03	0.40
2:H:151:THR:OG1	2:H:199:ASN:HB3	2.21	0.40
1:A:254:LYS:HA	1:A:254:LYS:HD3	1.67	0.40
1:B:337:LEU:HD13	2:C:32:TYR:CE2	2.56	0.40
3:L:23:CYS:HB2	3:L:35:TRP:CH2	2.57	0.40
1:A:249:GLN:NE2	1:A:307:LEU:HD21	2.35	0.40
2:H:19:LYS:HG3	2:H:81:GLN:HA	2.03	0.40
2:C:67:PHE:CE2	2:C:82:MET:HG2	2.57	0.40
2:C:68:THR:HB	2:C:81:GLN:HB3	2.03	0.40
1:B:205:ILE:HD11	1:B:225:PHE:CZ	2.56	0.40
1:B:252:SER:N	1:B:255:ASP:OD2	2.52	0.40
2:C:2:VAL:HG13	2:C:27:PHE:HD1	1.87	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)
3:L:70:ASP:O	3:D:24:ARG:NH2[1_455]	2.15	0.05

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	309/357 (87%)	286 (93%)	23 (7%)	0	100 100
1	B	309/357 (87%)	285 (92%)	24 (8%)	0	100 100
2	C	214/247 (87%)	202 (94%)	10 (5%)	2 (1%)	17 58
2	H	214/247 (87%)	205 (96%)	8 (4%)	1 (0%)	29 68
3	D	217/238 (91%)	209 (96%)	7 (3%)	1 (0%)	29 68
3	L	217/238 (91%)	208 (96%)	9 (4%)	0	100 100
All	All	1480/1684 (88%)	1395 (94%)	81 (6%)	4 (0%)	41 75

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	96	TYR
2	C	96	TYR
2	C	12	VAL
3	D	110	VAL

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	267/309 (86%)	263 (98%)	4 (2%)	65 84
1	B	268/309 (87%)	267 (100%)	1 (0%)	91 97
2	C	182/209 (87%)	181 (100%)	1 (0%)	88 95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	H	182/209 (87%)	182 (100%)	0	100 100
3	D	194/209 (93%)	193 (100%)	1 (0%)	88 95
3	L	194/209 (93%)	190 (98%)	4 (2%)	53 79
All	All	1287/1454 (88%)	1276 (99%)	11 (1%)	78 90

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	221	LEU
1	A	251	SER
1	A	292	CYS
1	A	321	MET
1	B	56	HIS
3	L	17	ASP
3	L	134	CYS
3	L	142	ARG
3	L	194	CYS
2	C	19	LYS
3	D	194	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	39	GLN
3	L	18	GLN
3	L	38	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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	313/357 (87%)	-0.40	1 (0%) 94 89	9, 31, 69, 85	0
1	B	313/357 (87%)	-0.20	7 (2%) 62 48	15, 35, 93, 135	0
2	C	216/247 (87%)	-0.19	3 (1%) 75 62	12, 39, 72, 84	0
2	H	216/247 (87%)	-0.47	1 (0%) 91 84	9, 26, 53, 88	0
3	D	219/238 (92%)	-0.34	0 100 100	12, 31, 64, 90	0
3	L	219/238 (92%)	-0.47	0 100 100	9, 28, 50, 67	0
All	All	1496/1684 (88%)	-0.34	12 (0%) 86 75	9, 31, 69, 135	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	15	GLY	3.4
1	B	279	SER	3.1
2	C	128	SER	2.9
1	B	305	CYS	2.8
1	B	301	ALA	2.7
2	H	133	GLY	2.7
2	C	133	GLY	2.6
1	B	269	SER	2.6
1	B	273	THR	2.5
1	B	277	SER	2.4
1	B	302	LYS	2.2
1	A	251	SER	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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.