



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2024 – 04:26 PM EDT

PDB ID : 3NN8
Title : Crystal structure of engineered antibody fragment based on 3D5
Authors : Lieberman, R.L.; Maynard, J.A.; Drury, J.E.; Pai, J.; Culver, J.A.
Deposited on : 2010-06-23
Resolution : 3.10 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 : 2.36
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) : 2.36

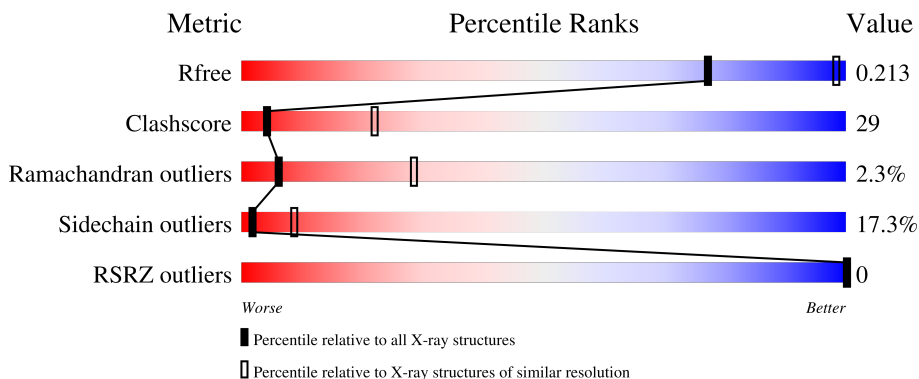
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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

Mol	Chain	Length	Quality of chain
1	A	256	
1	B	256	
1	C	256	
1	D	256	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7272 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 Engineered scFv.

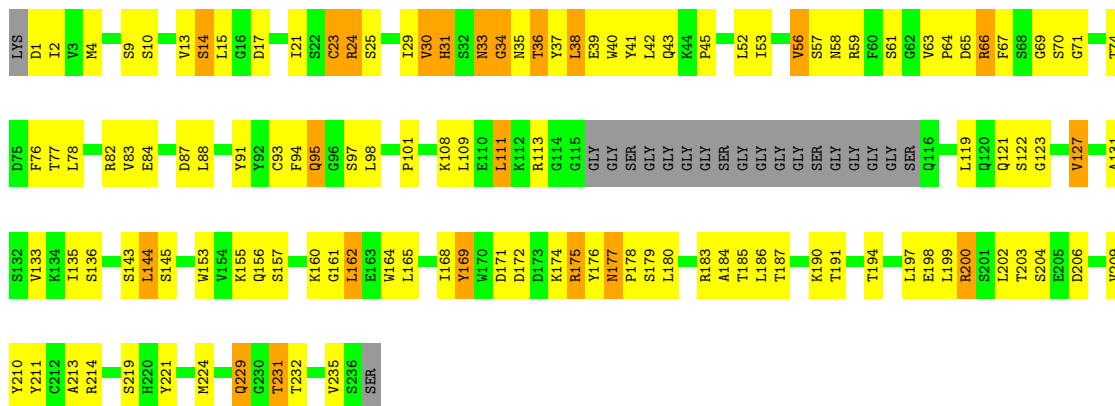
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	236	Total 1812	C 1138	N 308	O 359	S 7	0	0	0
1	B	238	Total 1827	C 1147	N 311	O 362	S 7	0	0	0
1	C	236	Total 1812	C 1138	N 308	O 359	S 7	0	0	0
1	D	237	Total 1821	C 1144	N 310	O 360	S 7	0	0	0

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.

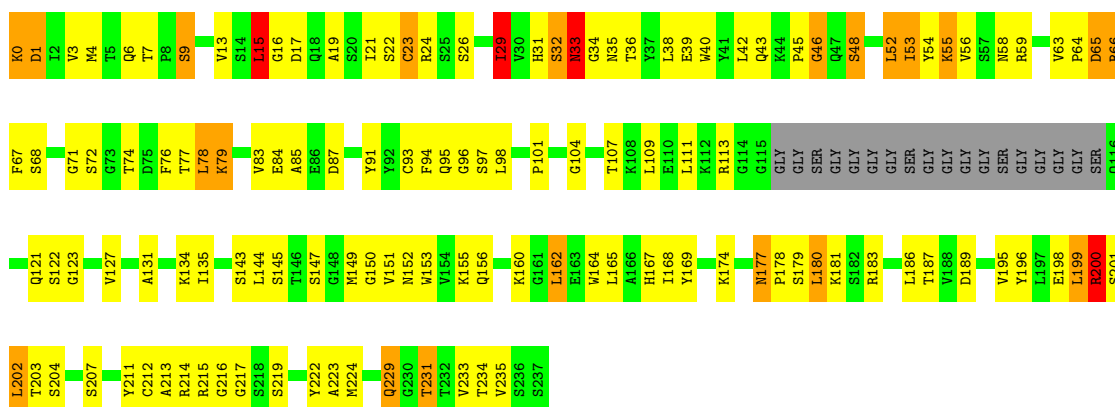
- Molecule 1: Engineered scFv

Chain A: 



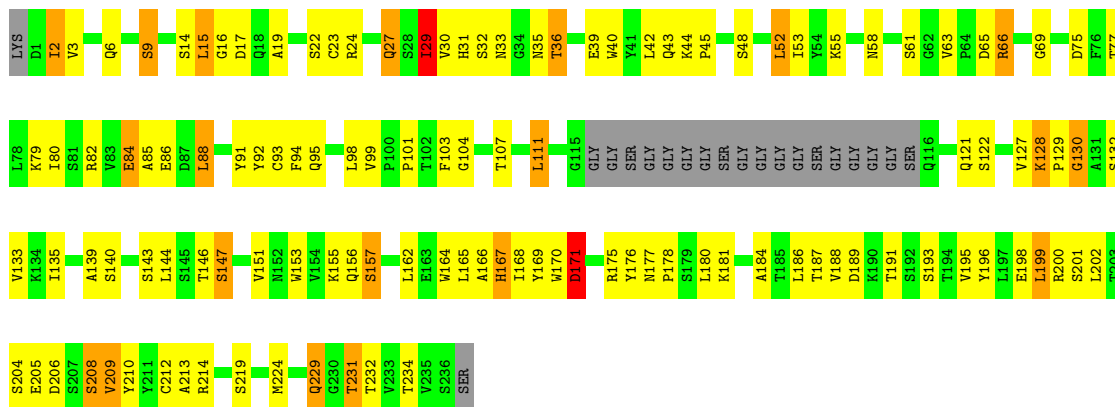
- Molecule 1: Engineered scFv

Chain B: 

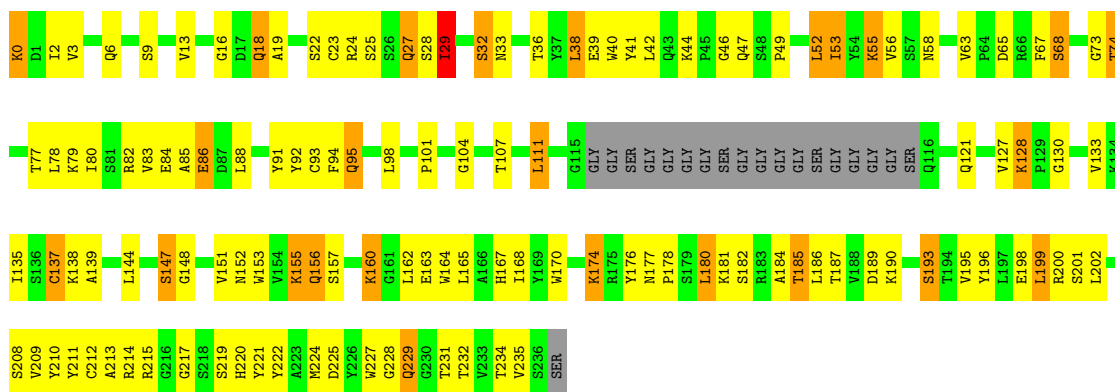


- Molecule 1: Engineered scFv

Chain C: 



● Molecule 1: Engineered scFv



4 Data and refinement statistics i

Property	Value	Source
Space group	F 2 3	Depositor
Cell constants a, b, c, α , β , γ	266.64Å 266.64Å 266.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	154.30 – 3.10 19.87 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (154.30-3.10) 100.0 (19.87-3.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.79 (at 3.09Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.183 , 0.238 0.195 , 0.213	Depositor DCC
R_{free} test set	1439 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	35.1	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , -6.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.469 for k,h,-l	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7272	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.76	0/1853	0.85	1/2510 (0.0%)
1	B	0.78	0/1868	0.87	5/2529 (0.2%)
1	C	0.77	0/1853	0.85	2/2510 (0.1%)
1	D	0.78	1/1862 (0.1%)	0.90	3/2521 (0.1%)
All	All	0.77	1/7436 (0.0%)	0.87	11/10070 (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	B	0	1
1	C	0	2
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	137	CYS	CB-SG	-5.33	1.73	1.81

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	46	GLY	N-CA-C	-6.97	95.66	113.10
1	D	23	CYS	CA-CB-SG	-6.92	101.54	114.00
1	B	23	CYS	CA-CB-SG	-6.88	101.62	114.00
1	C	23	CYS	CA-CB-SG	-6.26	102.73	114.00
1	B	201	SER	N-CA-C	-6.21	94.22	111.00
1	D	182	SER	N-CA-C	-6.16	94.38	111.00
1	A	23	CYS	CA-CB-SG	-6.15	102.93	114.00
1	B	15	LEU	CA-CB-CG	5.73	128.48	115.30
1	C	171	ASP	C-N-CA	-5.17	108.77	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	200	ARG	N-CA-C	-5.14	97.13	111.00
1	D	46	GLY	N-CA-C	-5.01	100.57	113.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	200	ARG	Peptide
1	C	130	GLY	Peptide
1	C	45	PRO	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	1812	0	1767	109	0
1	B	1827	0	1785	119	0
1	C	1812	0	1767	99	0
1	D	1821	0	1780	99	0
All	All	7272	0	7099	423	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 29.

All (423) 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:D:156:GLN:HG3	1:D:162:LEU:HD12	1.29	1.08
1:A:24:ARG:NH1	1:A:24:ARG:HB2	1.74	1.01
1:A:121:GLN:HB3	1:A:231:THR:HG22	1.40	1.01
1:B:29:ILE:HD11	1:B:95:GLN:HG3	1.46	0.97
1:C:121:GLN:H	1:C:229:GLN:HE22	1.07	0.96
1:B:149:MET:SD	1:B:216:GLY:HA2	2.10	0.92
1:B:13:VAL:HG21	1:B:109:LEU:HD11	1.53	0.91
1:B:121:GLN:HB3	1:B:231:THR:HG22	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:SER:HA	1:A:69:GLY:HA3	1.55	0.88
1:B:199:LEU:CD1	1:B:202:LEU:HD23	2.07	0.85
1:C:6:GLN:NE2	1:C:93:CYS:H	1.74	0.84
1:C:121:GLN:HB3	1:C:231:THR:HG22	1.61	0.83
1:D:55:LYS:O	1:D:55:LYS:HG3	1.78	0.83
1:B:6:GLN:HE21	1:B:104:GLY:HA3	1.43	0.82
1:A:13:VAL:HG21	1:A:109:LEU:HD11	1.59	0.82
1:A:24:ARG:HB2	1:A:24:ARG:HH11	1.41	0.82
1:B:199:LEU:HD13	1:B:202:LEU:HD23	1.62	0.82
1:C:121:GLN:H	1:C:229:GLN:NE2	1.76	0.82
1:A:133:VAL:HG22	1:A:202:LEU:HD11	1.63	0.81
1:B:217:GLY:HA3	1:B:222:TYR:CD1	2.16	0.81
1:C:128:LYS:H	1:C:128:LYS:NZ	1.80	0.80
1:D:156:GLN:HG3	1:D:162:LEU:CD1	2.09	0.79
1:B:43:GLN:HE22	1:B:156:GLN:HE22	1.30	0.79
1:B:32:SER:HA	1:B:33:ASN:C	2.05	0.77
1:A:13:VAL:HG11	1:A:83:VAL:HG21	1.66	0.77
1:D:52:LEU:HA	1:D:63:VAL:HG21	1.67	0.76
1:D:121:GLN:H	1:D:229:GLN:HE22	1.33	0.76
1:B:177:ASN:ND2	1:B:178:PRO:HD2	2.01	0.76
1:D:6:GLN:NE2	1:D:104:GLY:HA3	2.01	0.76
1:C:177:ASN:HD22	1:C:178:PRO:HD2	1.51	0.76
1:D:6:GLN:HE22	1:D:93:CYS:H	1.33	0.76
1:C:33:ASN:ND2	1:C:35:ASN:HB2	2.02	0.75
1:D:165:LEU:HD22	1:D:180:LEU:HD21	1.66	0.75
1:A:88:LEU:HD11	1:A:111:LEU:HD12	1.68	0.75
1:C:6:GLN:HE22	1:C:93:CYS:H	1.33	0.74
1:B:94:PHE:CZ	1:B:101:PRO:HB2	2.22	0.74
1:D:6:GLN:NE2	1:D:93:CYS:H	1.86	0.74
1:A:94:PHE:CZ	1:A:101:PRO:HB2	2.22	0.74
1:D:42:LEU:HB2	1:D:52:LEU:HD21	1.69	0.74
1:B:24:ARG:HB2	1:B:24:ARG:NH1	2.03	0.73
1:D:121:GLN:HE21	1:D:231:THR:HG22	1.53	0.73
1:A:29:ILE:HD12	1:A:95:GLN:HG3	1.70	0.72
1:B:177:ASN:HD22	1:B:178:PRO:HD2	1.53	0.72
1:D:121:GLN:H	1:D:229:GLN:NE2	1.86	0.72
1:A:229:GLN:H	1:A:229:GLN:NE2	1.87	0.72
1:B:177:ASN:HD22	1:B:178:PRO:CD	2.01	0.72
1:A:127:VAL:HG21	1:A:133:VAL:CG1	2.20	0.72
1:B:199:LEU:CD1	1:B:202:LEU:CD2	2.67	0.72
1:B:229:GLN:H	1:B:229:GLN:NE2	1.88	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:LEU:HD22	1:C:180:LEU:HD11	1.73	0.70
1:A:122:SER:HB3	1:A:136:SER:OG	1.91	0.70
1:A:157:SER:HB2	1:A:160:LYS:HB2	1.72	0.70
1:B:199:LEU:HD12	1:B:202:LEU:CD2	2.21	0.70
1:B:229:GLN:HE21	1:B:229:GLN:N	1.88	0.70
1:C:52:LEU:HA	1:C:63:VAL:HG21	1.75	0.69
1:D:156:GLN:CG	1:D:162:LEU:HD12	2.18	0.69
1:C:6:GLN:NE2	1:C:104:GLY:HA3	2.08	0.69
1:B:214:ARG:O	1:B:224:MET:HA	1.91	0.69
1:B:217:GLY:HA2	1:B:222:TYR:H	1.58	0.69
1:A:214:ARG:O	1:A:224:MET:HA	1.93	0.69
1:D:0:LYS:NZ	1:D:0:LYS:HB2	2.08	0.69
1:B:177:ASN:HD22	1:B:178:PRO:N	1.91	0.69
1:A:229:GLN:NE2	1:A:229:GLN:N	2.40	0.68
1:D:177:ASN:HD22	1:D:178:PRO:HD2	1.58	0.68
1:D:88:LEU:CD1	1:D:111:LEU:HD22	2.23	0.68
1:A:10:SER:O	1:A:108:LYS:O	2.11	0.68
1:D:2:ILE:HG21	1:D:29:ILE:HD11	1.73	0.68
1:A:24:ARG:HH11	1:A:24:ARG:CB	2.06	0.68
1:D:121:GLN:NE2	1:D:231:THR:HG22	2.09	0.68
1:C:170:TRP:C	1:C:171:ASP:O	2.24	0.67
1:B:66:ARG:NH1	1:B:87:ASP:OD1	2.28	0.67
1:D:27:GLN:HG3	1:D:28:SER:N	2.09	0.67
1:D:157:SER:HB2	1:D:160:LYS:HB2	1.77	0.67
1:A:30:VAL:HG23	1:A:36:THR:HG22	1.75	0.67
1:D:128:LYS:NZ	1:D:128:LYS:H	1.93	0.67
1:A:168:ILE:HB	1:A:186:LEU:HD13	1.77	0.66
1:A:71:GLY:HA3	1:A:76:PHE:HA	1.77	0.66
1:A:185:THR:HG23	1:A:200:ARG:HH22	1.61	0.65
1:B:183:ARG:HB3	1:B:200:ARG:O	1.96	0.65
1:B:29:ILE:CD1	1:B:95:GLN:HG3	2.25	0.65
1:A:122:SER:O	1:A:231:THR:HB	1.97	0.65
1:A:202:LEU:HB3	1:A:235:VAL:HG21	1.78	0.65
1:A:229:GLN:N	1:A:229:GLN:HE21	1.95	0.64
1:C:129:PRO:O	1:C:202:LEU:O	2.15	0.64
1:A:14:SER:O	1:A:17:ASP:HB2	1.97	0.64
1:A:95:GLN:NE2	1:A:98:LEU:H	1.96	0.64
1:B:21:ILE:HD12	1:B:78:LEU:HD23	1.80	0.64
1:B:32:SER:HA	1:B:33:ASN:O	1.98	0.64
1:D:185:THR:HB	1:D:200:ARG:HH22	1.62	0.63
1:D:185:THR:HB	1:D:200:ARG:NH2	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:214:ARG:O	1:D:224:MET:HA	1.99	0.63
1:C:40:TRP:HB2	1:C:53:ILE:HB	1.81	0.62
1:B:31:HIS:HB3	1:B:33:ASN:HD21	1.64	0.62
1:B:54:TYR:O	1:B:58:ASN:HB2	2.00	0.62
1:C:128:LYS:H	1:C:128:LYS:HZ1	1.46	0.62
1:B:95:GLN:HE21	1:B:97:SER:H	1.48	0.62
1:B:229:GLN:NE2	1:B:229:GLN:N	2.48	0.62
1:B:199:LEU:HD13	1:B:202:LEU:CD2	2.29	0.61
1:B:121:GLN:NE2	1:B:231:THR:HG22	2.16	0.61
1:C:19:ALA:HB3	1:C:80:ILE:HB	1.82	0.61
1:D:88:LEU:HD11	1:D:111:LEU:HD22	1.83	0.60
1:B:42:LEU:HB2	1:B:52:LEU:HD21	1.83	0.60
1:A:121:GLN:HB3	1:A:231:THR:CG2	2.24	0.60
1:C:133:VAL:HB	1:C:202:LEU:HD11	1.83	0.60
1:A:177:ASN:ND2	1:A:179:SER:H	2.00	0.60
1:B:66:ARG:HH12	1:B:84:GLU:HB2	1.66	0.60
1:A:24:ARG:HB2	1:A:24:ARG:CZ	2.29	0.60
1:B:9:SER:O	1:B:107:THR:HA	2.03	0.59
1:C:132:SER:HA	1:C:200:ARG:HA	1.85	0.59
1:B:52:LEU:HA	1:B:63:VAL:HG21	1.84	0.59
1:C:33:ASN:HD21	1:C:35:ASN:HB2	1.68	0.59
1:A:155:LYS:HB3	1:A:165:LEU:HD11	1.84	0.59
1:A:29:ILE:O	1:A:29:ILE:HG22	2.00	0.58
1:A:206:ASP:O	1:A:210:TYR:OH	2.18	0.58
1:B:177:ASN:ND2	1:B:179:SER:H	2.02	0.58
1:B:0:LYS:HD3	1:B:1:ASP:H	1.69	0.58
1:C:27:GLN:HE21	1:C:27:GLN:HA	1.69	0.58
1:D:139:ALA:O	1:D:193:SER:HB3	2.04	0.58
1:C:128:LYS:H	1:C:128:LYS:HZ2	1.51	0.58
1:C:42:LEU:HB2	1:C:52:LEU:HD21	1.86	0.57
1:A:42:LEU:HD13	1:A:91:TYR:CZ	2.39	0.57
1:D:95:GLN:NE2	1:D:98:LEU:H	2.02	0.57
1:C:214:ARG:O	1:C:224:MET:HA	2.04	0.56
1:D:185:THR:CB	1:D:200:ARG:HH22	2.19	0.56
1:B:24:ARG:HB2	1:B:24:ARG:CZ	2.35	0.56
1:A:33:ASN:HD22	1:A:35:ASN:H	1.53	0.56
1:B:155:LYS:HB3	1:B:165:LEU:HD11	1.87	0.56
1:C:147:SER:HA	1:C:170:TRP:CD2	2.41	0.56
1:A:53:ILE:HD13	1:A:78:LEU:CD1	2.36	0.56
1:C:2:ILE:HD13	1:C:2:ILE:C	2.25	0.56
1:A:127:VAL:HG21	1:A:133:VAL:HG12	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:GLN:HE21	1:D:98:LEU:H	1.53	0.56
1:B:168:ILE:HB	1:B:186:LEU:HD13	1.87	0.56
1:D:127:VAL:HG23	1:D:235:VAL:HG22	1.88	0.55
1:B:24:ARG:HH11	1:B:24:ARG:CB	2.19	0.55
1:D:6:GLN:HE21	1:D:104:GLY:HA3	1.69	0.55
1:D:184:ALA:HA	1:D:198:GLU:O	2.06	0.55
1:B:24:ARG:NH1	1:B:24:ARG:CB	2.69	0.55
1:B:94:PHE:CE1	1:B:101:PRO:HB2	2.42	0.55
1:D:24:ARG:HA	1:D:74:THR:O	2.07	0.55
1:C:33:ASN:HD22	1:C:35:ASN:HD22	1.54	0.55
1:D:25:SER:OG	1:D:74:THR:HA	2.07	0.54
1:D:18:GLN:HE22	1:D:79:LYS:HD2	1.72	0.54
1:A:40:TRP:CZ3	1:A:93:CYS:HB3	2.42	0.54
1:B:65:ASP:OD1	1:B:65:ASP:N	2.38	0.54
1:B:121:GLN:HB3	1:B:231:THR:CG2	2.32	0.54
1:D:137:CYS:HB2	1:D:153:TRP:CZ2	2.42	0.54
1:B:32:SER:CA	1:B:33:ASN:O	2.55	0.54
1:B:152:ASN:OD1	1:B:167:HIS:HB2	2.07	0.54
1:C:213:ALA:HB1	1:C:224:MET:HB3	1.89	0.54
1:A:33:ASN:ND2	1:A:35:ASN:H	2.06	0.53
1:D:209:VAL:HA	1:D:232:THR:HA	1.88	0.53
1:B:122:SER:O	1:B:231:THR:HB	2.08	0.53
1:C:121:GLN:HB3	1:C:231:THR:CG2	2.36	0.53
1:C:143:SER:HB3	1:C:146:THR:HG23	1.90	0.53
1:A:172:ASP:OD2	1:A:174:LYS:HE3	2.09	0.53
1:C:121:GLN:N	1:C:229:GLN:HE22	1.91	0.53
1:D:164:TRP:CE3	1:D:177:ASN:HB2	2.44	0.53
1:D:55:LYS:O	1:D:55:LYS:CG	2.52	0.53
1:B:156:GLN:HB2	1:B:162:LEU:HD12	1.91	0.53
1:A:31:HIS:HB3	1:A:33:ASN:N	2.25	0.52
1:A:101:PRO:HG2	1:A:164:TRP:CG	2.43	0.52
1:B:13:VAL:HG21	1:B:109:LEU:CD1	2.33	0.52
1:B:32:SER:N	1:B:33:ASN:O	2.42	0.52
1:B:101:PRO:HG2	1:B:164:TRP:CG	2.44	0.52
1:B:39:GLU:HA	1:B:53:ILE:O	2.09	0.52
1:B:1:ASP:OD2	1:B:1:ASP:N	2.42	0.52
1:D:88:LEU:HD13	1:D:111:LEU:HD22	1.91	0.52
1:A:177:ASN:HD22	1:A:179:SER:H	1.58	0.52
1:A:213:ALA:HB1	1:A:224:MET:HB3	1.92	0.52
1:B:53:ILE:HA	1:B:58:ASN:O	2.10	0.52
1:B:72:SER:O	1:B:76:PHE:CE1	2.63	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:GLN:HE21	1:A:97:SER:H	1.58	0.52
1:C:121:GLN:NE2	1:C:231:THR:HG22	2.25	0.52
1:A:29:ILE:HD12	1:A:95:GLN:CG	2.40	0.51
1:C:15:LEU:HD13	1:C:111:LEU:HD11	1.91	0.51
1:A:175:ARG:CG	1:A:175:ARG:HH11	2.23	0.51
1:A:95:GLN:HE21	1:A:97:SER:N	2.09	0.51
1:B:215:ARG:O	1:B:223:ALA:O	2.29	0.51
1:D:19:ALA:HB3	1:D:80:ILE:HD12	1.93	0.51
1:B:217:GLY:O	1:B:219:SER:N	2.44	0.51
1:B:199:LEU:HD12	1:B:202:LEU:HD23	1.86	0.51
1:D:153:TRP:HE1	1:D:195:VAL:HG11	1.74	0.51
1:B:55:LYS:HB3	1:B:58:ASN:HD22	1.75	0.51
1:B:143:SER:C	1:B:145:SER:H	2.13	0.51
1:C:170:TRP:CG	1:C:171:ASP:N	2.79	0.51
1:D:155:LYS:HE3	1:D:208:SER:OG	2.11	0.51
1:A:183:ARG:O	1:A:200:ARG:HB2	2.11	0.50
1:D:39:GLU:HA	1:D:53:ILE:O	2.10	0.50
1:D:94:PHE:CZ	1:D:101:PRO:HB2	2.47	0.50
1:B:217:GLY:HA3	1:B:222:TYR:CE1	2.47	0.50
1:A:176:TYR:HE1	1:A:186:LEU:H	1.59	0.50
1:A:177:ASN:HD22	1:A:178:PRO:N	2.10	0.50
1:B:40:TRP:CZ3	1:B:93:CYS:HB3	2.47	0.50
1:B:127:VAL:HG13	1:B:131:ALA:HB3	1.93	0.50
1:D:67:PHE:CE1	1:D:80:ILE:HG12	2.47	0.50
1:D:128:LYS:H	1:D:128:LYS:HZ2	1.60	0.50
1:C:6:GLN:HA	1:C:22:SER:O	2.11	0.50
1:A:209:VAL:CG2	1:A:211:TYR:CE2	2.95	0.50
1:D:40:TRP:CH2	1:D:93:CYS:HB3	2.46	0.50
1:B:204:SER:HA	1:B:235:VAL:HB	1.93	0.50
1:B:121:GLN:HE21	1:B:231:THR:HG22	1.75	0.49
1:B:4:MET:HE3	1:B:23:CYS:HB3	1.94	0.49
1:D:3:VAL:O	1:D:25:SER:HA	2.11	0.49
1:D:53:ILE:HA	1:D:58:ASN:O	2.12	0.49
1:B:64:PRO:HB2	1:B:66:ARG:HE	1.77	0.49
1:C:53:ILE:HA	1:C:58:ASN:O	2.12	0.49
1:D:40:TRP:CZ3	1:D:93:CYS:HB3	2.47	0.49
1:B:31:HIS:HB3	1:B:33:ASN:ND2	2.27	0.49
1:D:189:ASP:HB2	1:D:196:TYR:HE2	1.77	0.49
1:B:42:LEU:HD13	1:B:91:TYR:CZ	2.47	0.49
1:C:168:ILE:HG22	1:C:186:LEU:HD13	1.95	0.49
1:D:165:LEU:HD11	1:D:210:TYR:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:GLN:NE2	1:B:104:GLY:HA3	2.21	0.49
1:C:151:VAL:CG1	1:C:212:CYS:HB2	2.43	0.49
1:A:209:VAL:HA	1:A:232:THR:HA	1.95	0.49
1:C:139:ALA:CB	1:C:144:LEU:HD21	2.43	0.48
1:D:58:ASN:N	1:D:58:ASN:HD22	2.11	0.48
1:A:180:LEU:HD13	1:A:184:ALA:HB2	1.95	0.48
1:A:143:SER:O	1:A:145:SER:N	2.46	0.48
1:B:152:ASN:O	1:B:212:CYS:HA	2.13	0.48
1:A:4:MET:HE3	1:A:23:CYS:HB3	1.96	0.48
1:A:143:SER:C	1:A:145:SER:H	2.16	0.48
1:C:155:LYS:HB3	1:C:165:LEU:HD11	1.96	0.48
1:D:133:VAL:HG22	1:D:202:LEU:HD11	1.95	0.48
1:A:43:GLN:HE22	1:A:156:GLN:HE22	1.61	0.48
1:B:59:ARG:HD3	1:B:67:PHE:O	2.13	0.48
1:C:165:LEU:HD11	1:C:210:TYR:CE1	2.48	0.48
1:A:175:ARG:CG	1:A:175:ARG:NH1	2.77	0.48
1:C:122:SER:O	1:C:231:THR:HB	2.14	0.48
1:B:177:ASN:HD22	1:B:177:ASN:C	2.16	0.48
1:D:92:TYR:CD2	1:D:162:LEU:HD22	2.48	0.48
1:D:49:PRO:HG2	1:D:227:TRP:CZ3	2.49	0.48
1:D:148:GLY:HA3	1:D:217:GLY:HA2	1.96	0.48
1:A:127:VAL:HG13	1:A:131:ALA:HB3	1.94	0.47
1:A:38:LEU:HD22	1:A:76:PHE:CG	2.50	0.47
1:B:3:VAL:HG12	1:B:26:SER:HB3	1.95	0.47
1:C:9:SER:O	1:C:107:THR:HA	2.13	0.47
1:C:40:TRP:CZ3	1:C:93:CYS:HB3	2.49	0.47
1:D:29:ILE:HG13	1:D:95:GLN:HG3	1.95	0.47
1:D:84:GLU:O	1:D:85:ALA:C	2.52	0.47
1:A:113:ARG:NH2	1:C:229:GLN:O	2.47	0.47
1:D:121:GLN:N	1:D:229:GLN:HE22	2.08	0.47
1:B:15:LEU:HA	1:B:16:GLY:HA2	1.56	0.47
1:C:29:ILE:HD11	1:C:95:GLN:HG3	1.96	0.47
1:C:16:GLY:HA2	1:C:82:ARG:HG3	1.94	0.47
1:D:151:VAL:HG21	1:D:195:VAL:HG21	1.97	0.47
1:C:40:TRP:CH2	1:C:93:CYS:HB3	2.49	0.47
1:C:66:ARG:O	1:C:80:ILE:HA	2.14	0.47
1:D:52:LEU:HD12	1:D:63:VAL:HG22	1.97	0.47
1:A:25:SER:CB	1:A:29:ILE:HD11	2.45	0.47
1:A:95:GLN:HE21	1:A:98:LEU:H	1.60	0.47
1:B:213:ALA:HB1	1:B:224:MET:HB3	1.97	0.47
1:C:39:GLU:HA	1:C:53:ILE:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:TRP:CD1	1:D:186:LEU:HD21	2.49	0.47
1:A:52:LEU:HA	1:A:63:VAL:HG21	1.96	0.46
1:C:156:GLN:HG3	1:C:162:LEU:HD12	1.98	0.46
1:B:38:LEU:HD23	1:B:56:VAL:HA	1.98	0.46
1:B:144:LEU:HD23	1:B:144:LEU:HA	1.79	0.46
1:C:6:GLN:HE21	1:C:104:GLY:HA3	1.77	0.46
1:C:164:TRP:CE3	1:C:177:ASN:HB2	2.51	0.46
1:D:164:TRP:CZ3	1:D:177:ASN:HB2	2.50	0.46
1:A:155:LYS:HD3	1:A:165:LEU:HD21	1.98	0.46
1:A:171:ASP:O	1:A:172:ASP:HB3	2.15	0.46
1:D:16:GLY:HA2	1:D:82:ARG:HG3	1.97	0.46
1:A:21:ILE:HD12	1:A:78:LEU:HD23	1.98	0.46
1:C:14:SER:N	1:C:17:ASP:OD1	2.46	0.46
1:C:94:PHE:CZ	1:C:101:PRO:HB2	2.50	0.46
1:D:209:VAL:HG22	1:D:211:TYR:CE2	2.51	0.46
1:C:101:PRO:HG2	1:C:164:TRP:CG	2.50	0.46
1:C:170:TRP:CD1	1:C:170:TRP:N	2.82	0.46
1:B:151:VAL:HG21	1:B:195:VAL:HG21	1.97	0.46
1:A:153:TRP:CD1	1:A:186:LEU:HD21	2.51	0.46
1:D:44:LYS:HD3	1:D:86:GLU:O	2.15	0.46
1:D:68:SER:O	1:D:78:LEU:HD12	2.16	0.46
1:C:31:HIS:ND1	1:C:33:ASN:OD1	2.49	0.46
1:D:168:ILE:HB	1:D:186:LEU:HD13	1.97	0.46
1:C:153:TRP:CD1	1:C:186:LEU:HD21	2.50	0.46
1:D:13:VAL:HG21	1:D:83:VAL:HG11	1.98	0.46
1:C:29:ILE:CD1	1:C:95:GLN:HG3	2.46	0.45
1:A:53:ILE:HA	1:A:58:ASN:O	2.16	0.45
1:A:156:GLN:HB2	1:A:162:LEU:CD1	2.46	0.45
1:C:127:VAL:HG21	1:C:202:LEU:HD13	1.97	0.45
1:A:95:GLN:O	1:A:95:GLN:CD	2.54	0.45
1:B:207:SER:HA	1:B:233:VAL:O	2.16	0.45
1:C:177:ASN:ND2	1:C:178:PRO:HD2	2.26	0.45
1:C:189:ASP:HB2	1:C:196:TYR:HE2	1.82	0.45
1:B:121:GLN:HE21	1:B:231:THR:CG2	2.29	0.45
1:A:136:SER:HB2	1:A:194:THR:CG2	2.47	0.45
1:A:169:TYR:HB3	1:A:171:ASP:OD2	2.17	0.45
1:B:121:GLN:NE2	1:B:231:THR:CG2	2.80	0.45
1:A:204:SER:HA	1:A:235:VAL:HB	1.98	0.45
1:D:38:LEU:HG	1:D:39:GLU:N	2.32	0.45
1:B:13:VAL:HG11	1:B:83:VAL:HG21	1.99	0.45
1:D:153:TRP:HE1	1:D:195:VAL:CG1	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:SER:HB2	1:B:77:THR:HG22	1.98	0.45
1:B:38:LEU:HG	1:B:39:GLU:N	2.32	0.45
1:C:6:GLN:OE1	1:C:91:TYR:O	2.35	0.44
1:C:128:LYS:HZ1	1:C:128:LYS:N	2.15	0.44
1:C:199:LEU:HD13	1:C:202:LEU:HD21	1.99	0.44
1:D:221:TYR:N	1:D:221:TYR:CD2	2.85	0.44
1:A:13:VAL:HG21	1:A:109:LEU:CD1	2.39	0.44
1:A:95:GLN:NE2	1:A:95:GLN:O	2.50	0.44
1:C:184:ALA:HA	1:C:198:GLU:O	2.18	0.44
1:D:147:SER:HA	1:D:170:TRP:CD2	2.52	0.44
1:B:153:TRP:CD1	1:B:186:LEU:HD21	2.53	0.44
1:C:157:SER:CA	1:C:208:SER:HB2	2.47	0.44
1:C:209:VAL:HA	1:C:232:THR:HA	1.98	0.44
1:A:41:TYR:O	1:A:91:TYR:HA	2.17	0.44
1:B:15:LEU:HD22	1:B:111:LEU:HD11	1.99	0.44
1:B:95:GLN:HE21	1:B:97:SER:N	2.13	0.44
1:D:9:SER:O	1:D:107:THR:HA	2.17	0.44
1:D:151:VAL:CG1	1:D:212:CYS:HB2	2.47	0.44
1:B:199:LEU:HD12	1:B:202:LEU:HD21	2.00	0.44
1:D:39:GLU:HB3	1:D:41:TYR:CE2	2.52	0.44
1:A:39:GLU:HA	1:A:53:ILE:O	2.18	0.44
1:A:184:ALA:HA	1:A:198:GLU:O	2.18	0.44
1:A:121:GLN:NE2	1:A:231:THR:HG22	2.33	0.44
1:B:45:PRO:HA	1:B:46:GLY:HA2	1.76	0.44
1:C:69:GLY:HA2	1:C:77:THR:O	2.17	0.44
1:B:6:GLN:HA	1:B:22:SER:O	2.18	0.44
1:B:4:MET:CE	1:B:23:CYS:HB3	2.47	0.43
1:C:94:PHE:CE1	1:C:101:PRO:HB2	2.52	0.43
1:D:28:SER:HA	1:D:74:THR:HG22	1.99	0.43
1:D:199:LEU:HB3	1:D:202:LEU:HD21	1.99	0.43
1:D:6:GLN:HA	1:D:22:SER:O	2.18	0.43
1:B:59:ARG:NH1	1:B:67:PHE:O	2.46	0.43
1:C:44:LYS:HG2	1:C:88:LEU:O	2.18	0.43
1:D:101:PRO:HG2	1:D:164:TRP:CG	2.53	0.43
1:B:113:ARG:O	1:D:231:THR:HA	2.18	0.43
1:B:121:GLN:CB	1:B:231:THR:HG22	2.37	0.43
1:C:229:GLN:NE2	1:C:229:GLN:H	2.15	0.43
1:C:43:GLN:HE22	1:C:156:GLN:NE2	2.17	0.43
1:A:121:GLN:CB	1:A:231:THR:HG22	2.29	0.43
1:C:22:SER:CB	1:C:77:THR:HG22	2.49	0.43
1:A:135:ILE:HD11	1:A:197:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ARG:HD3	1:A:67:PHE:O	2.19	0.43
1:D:29:ILE:HD12	1:D:29:ILE:HA	1.79	0.43
1:D:95:GLN:HE21	1:D:98:LEU:N	2.16	0.43
1:D:130:GLY:N	1:D:202:LEU:O	2.51	0.43
1:D:219:SER:O	1:D:220:HIS:HB2	2.19	0.43
1:A:202:LEU:HB3	1:A:235:VAL:CG2	2.48	0.42
1:B:48:SER:HA	1:B:211:TYR:CE1	2.54	0.42
1:A:136:SER:HB2	1:A:194:THR:HG21	2.01	0.42
1:C:92:TYR:CD2	1:C:162:LEU:HD22	2.54	0.42
1:A:42:LEU:HD13	1:A:91:TYR:CE2	2.54	0.42
1:A:144:LEU:HD23	1:A:144:LEU:HA	1.66	0.42
1:B:95:GLN:NE2	1:B:98:LEU:H	2.17	0.42
1:C:180:LEU:HD23	1:C:180:LEU:HA	1.78	0.42
1:A:94:PHE:CE1	1:A:101:PRO:HB2	2.54	0.42
1:B:174:LYS:HG2	1:B:186:LEU:HB2	2.02	0.42
1:C:2:ILE:HD11	1:C:29:ILE:HD11	2.01	0.42
1:C:147:SER:HA	1:C:170:TRP:CE3	2.53	0.42
1:D:86:GLU:H	1:D:86:GLU:HG3	1.43	0.42
1:D:121:GLN:OE1	1:D:228:GLY:HA3	2.19	0.42
1:C:188:VAL:HG23	1:C:195:VAL:HG22	2.02	0.42
1:C:15:LEU:CD1	1:C:111:LEU:HD11	2.49	0.42
1:C:99:VAL:HA	1:C:101:PRO:HD3	2.02	0.42
1:C:155:LYS:HD3	1:C:208:SER:CB	2.49	0.42
1:C:165:LEU:HD23	1:C:165:LEU:HA	1.73	0.42
1:D:22:SER:CB	1:D:77:THR:HG22	2.49	0.42
1:A:175:ARG:NH1	1:A:175:ARG:HG2	2.35	0.42
1:A:177:ASN:HA	1:A:178:PRO:HD2	1.80	0.42
1:B:24:ARG:HH11	1:B:24:ARG:HB3	1.84	0.42
1:B:180:LEU:HD12	1:B:180:LEU:HA	1.70	0.42
1:A:33:ASN:ND2	1:A:34:GLY:H	2.18	0.42
1:B:84:GLU:O	1:B:85:ALA:C	2.58	0.42
1:C:2:ILE:HD13	1:C:3:VAL:N	2.35	0.42
1:C:130:GLY:O	1:C:201:SER:HA	2.20	0.42
1:C:139:ALA:HB2	1:C:144:LEU:HD21	2.02	0.42
1:C:156:GLN:HE21	1:C:156:GLN:HB3	1.66	0.42
1:D:42:LEU:HD13	1:D:91:TYR:CZ	2.55	0.42
1:D:176:TYR:HE1	1:D:186:LEU:H	1.67	0.42
1:C:95:GLN:NE2	1:C:98:LEU:H	2.17	0.42
1:C:206:ASP:C	1:C:208:SER:H	2.23	0.42
1:D:128:LYS:H	1:D:128:LYS:HZ1	1.66	0.42
1:B:19:ALA:O	1:B:79:LYS:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:ASP:HB2	1:B:196:TYR:HE2	1.85	0.42
1:C:15:LEU:HD13	1:C:111:LEU:CD1	2.50	0.42
1:C:30:VAL:HG12	1:C:36:THR:HB	2.02	0.42
1:C:167:HIS:ND1	1:C:167:HIS:C	2.73	0.42
1:A:177:ASN:HD22	1:A:177:ASN:C	2.22	0.41
1:B:15:LEU:H	1:B:15:LEU:CD2	2.32	0.41
1:C:103:PHE:CE1	1:C:162:LEU:HD23	2.55	0.41
1:A:71:GLY:CA	1:A:76:PHE:HA	2.48	0.41
1:A:174:LYS:NZ	1:D:174:LYS:NZ	2.68	0.41
1:D:40:TRP:HD1	1:D:53:ILE:CG2	2.33	0.41
1:A:66:ARG:NH1	1:A:87:ASP:OD2	2.53	0.41
1:A:37:TYR:CD1	1:A:221:TYR:HB3	2.55	0.41
1:B:17:ASP:O	1:B:83:VAL:HG23	2.20	0.41
1:B:33:ASN:O	1:B:35:ASN:N	2.53	0.41
1:B:63:VAL:HA	1:B:64:PRO:HD3	1.80	0.41
1:B:94:PHE:CZ	1:B:101:PRO:CB	3.00	0.41
1:B:150:GLY:HA3	1:B:167:HIS:HE1	1.86	0.41
1:B:199:LEU:CD1	1:B:202:LEU:HD21	2.48	0.41
1:B:32:SER:CA	1:B:33:ASN:C	2.84	0.41
1:C:166:ALA:HA	1:C:175:ARG:O	2.21	0.41
1:C:176:TYR:HE1	1:C:186:LEU:H	1.67	0.41
1:D:144:LEU:HD23	1:D:144:LEU:HA	1.74	0.41
1:D:152:ASN:OD1	1:D:167:HIS:HB3	2.20	0.41
1:A:15:LEU:HD21	1:A:111:LEU:HD11	2.03	0.41
1:A:180:LEU:HA	1:A:180:LEU:HD23	1.83	0.41
1:A:56:VAL:CG2	1:A:71:GLY:H	2.34	0.41
1:B:96:GLY:HA2	1:B:101:PRO:HB3	2.02	0.41
1:B:177:ASN:HD22	1:B:179:SER:H	1.67	0.41
1:A:40:TRP:CH2	1:A:93:CYS:HB3	2.55	0.41
1:A:66:ARG:HD3	1:A:82:ARG:O	2.21	0.41
1:B:29:ILE:HA	1:B:29:ILE:HD12	1.64	0.41
1:C:167:HIS:CD2	1:C:169:TYR:CZ	3.09	0.41
1:D:215:ARG:NH2	1:D:222:TYR:CD1	2.89	0.41
1:A:38:LEU:HD22	1:A:76:PHE:CB	2.51	0.41
1:A:156:GLN:HB2	1:A:162:LEU:HD13	2.03	0.41
1:C:6:GLN:HE22	1:C:93:CYS:N	2.09	0.40
1:A:109:LEU:HD12	1:A:109:LEU:HA	1.94	0.40
1:B:143:SER:C	1:B:145:SER:N	2.74	0.40
1:C:29:ILE:HA	1:C:29:ILE:HD12	1.82	0.40
1:C:84:GLU:O	1:C:85:ALA:C	2.59	0.40
1:D:213:ALA:HB1	1:D:224:MET:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:LEU:HD11	1:A:111:LEU:CD1	2.45	0.40
1:A:209:VAL:HG22	1:A:211:TYR:CE2	2.56	0.40
1:A:64:PRO:HG2	1:A:66:ARG:NH1	2.35	0.40
1:A:98:LEU:HD13	1:A:98:LEU:HA	1.89	0.40
1:B:134:LYS:HA	1:B:198:GLU:HA	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	232/256 (91%)	207 (89%)	17 (7%)	8 (3%)	3	21
1	B	234/256 (91%)	215 (92%)	13 (6%)	6 (3%)	5	26
1	C	232/256 (91%)	210 (90%)	18 (8%)	4 (2%)	9	36
1	D	233/256 (91%)	206 (88%)	24 (10%)	3 (1%)	12	42
All	All	931/1024 (91%)	838 (90%)	72 (8%)	21 (2%)	6	28

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	29	ILE
1	B	33	ASN
1	C	32	SER
1	C	171	ASP
1	A	161	GLY
1	B	32	SER
1	B	71	GLY
1	C	29	ILE
1	C	55	LYS
1	D	32	SER

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Mol	Chain	Res	Type
1	A	123	GLY
1	A	34	GLY
1	A	61	SER
1	A	70	SER
1	A	144	LEU
1	B	34	GLY
1	D	73	GLY
1	A	45	PRO
1	A	56	VAL
1	D	29	ILE
1	B	123	GLY

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	203/209 (97%)	171 (84%)	32 (16%)	2	11
1	B	205/209 (98%)	172 (84%)	33 (16%)	2	10
1	C	203/209 (97%)	166 (82%)	37 (18%)	1	7
1	D	204/209 (98%)	165 (81%)	39 (19%)	1	6
All	All	815/836 (98%)	674 (83%)	141 (17%)	2	9

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ASP
1	A	2	ILE
1	A	9	SER
1	A	14	SER
1	A	24	ARG
1	A	30	VAL
1	A	31	HIS
1	A	33	ASN
1	A	36	THR
1	A	38	LEU

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Mol	Chain	Res	Type
1	A	65	ASP
1	A	66	ARG
1	A	74	THR
1	A	77	THR
1	A	84	GLU
1	A	95	GLN
1	A	111	LEU
1	A	119	LEU
1	A	127	VAL
1	A	162	LEU
1	A	169	TYR
1	A	175	ARG
1	A	177	ASN
1	A	187	THR
1	A	190	LYS
1	A	191	THR
1	A	199	LEU
1	A	200	ARG
1	A	203	THR
1	A	219	SER
1	A	229	GLN
1	A	231	THR
1	B	0	LYS
1	B	1	ASP
1	B	7	THR
1	B	9	SER
1	B	15	LEU
1	B	29	ILE
1	B	33	ASN
1	B	36	THR
1	B	48	SER
1	B	52	LEU
1	B	53	ILE
1	B	55	LYS
1	B	65	ASP
1	B	66	ARG
1	B	68	SER
1	B	74	THR
1	B	78	LEU
1	B	79	LYS
1	B	135	ILE
1	B	147	SER

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Mol	Chain	Res	Type
1	B	160	LYS
1	B	162	LEU
1	B	169	TYR
1	B	177	ASN
1	B	180	LEU
1	B	181	LYS
1	B	187	THR
1	B	199	LEU
1	B	202	LEU
1	B	203	THR
1	B	229	GLN
1	B	231	THR
1	B	234	THR
1	C	2	ILE
1	C	9	SER
1	C	15	LEU
1	C	24	ARG
1	C	27	GLN
1	C	29	ILE
1	C	36	THR
1	C	48	SER
1	C	52	LEU
1	C	61	SER
1	C	65	ASP
1	C	66	ARG
1	C	75	ASP
1	C	79	LYS
1	C	84	GLU
1	C	86	GLU
1	C	88	LEU
1	C	111	LEU
1	C	128	LYS
1	C	135	ILE
1	C	140	SER
1	C	147	SER
1	C	157	SER
1	C	167	HIS
1	C	181	LYS
1	C	187	THR
1	C	191	THR
1	C	193	SER
1	C	199	LEU

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Mol	Chain	Res	Type
1	C	204	SER
1	C	205	GLU
1	C	208	SER
1	C	209	VAL
1	C	219	SER
1	C	229	GLN
1	C	231	THR
1	C	234	THR
1	D	0	LYS
1	D	18	GLN
1	D	27	GLN
1	D	29	ILE
1	D	32	SER
1	D	33	ASN
1	D	36	THR
1	D	38	LEU
1	D	47	GLN
1	D	52	LEU
1	D	53	ILE
1	D	55	LYS
1	D	56	VAL
1	D	65	ASP
1	D	68	SER
1	D	74	THR
1	D	86	GLU
1	D	95	GLN
1	D	111	LEU
1	D	128	LYS
1	D	135	ILE
1	D	138	LYS
1	D	147	SER
1	D	155	LYS
1	D	156	GLN
1	D	160	LYS
1	D	163	GLU
1	D	174	LYS
1	D	180	LEU
1	D	181	LYS
1	D	185	THR
1	D	187	THR
1	D	190	LYS
1	D	193	SER

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Mol	Chain	Res	Type
1	D	199	LEU
1	D	201	SER
1	D	225	ASP
1	D	229	GLN
1	D	234	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	43	GLN
1	A	47	GLN
1	A	95	GLN
1	A	177	ASN
1	A	229	GLN
1	B	6	GLN
1	B	33	ASN
1	B	58	ASN
1	B	95	GLN
1	B	156	GLN
1	B	177	ASN
1	B	229	GLN
1	C	6	GLN
1	C	27	GLN
1	C	35	ASN
1	C	43	GLN
1	C	58	ASN
1	C	95	GLN
1	C	167	HIS
1	C	229	GLN
1	D	6	GLN
1	D	18	GLN
1	D	43	GLN
1	D	58	ASN
1	D	95	GLN
1	D	116	GLN
1	D	156	GLN
1	D	167	HIS
1	D	229	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	236/256 (92%)	-0.29	0 100 100	16, 62, 120, 150	0
1	B	238/256 (92%)	-0.27	0 100 100	16, 64, 122, 158	0
1	C	236/256 (92%)	-0.24	0 100 100	15, 66, 142, 174	0
1	D	237/256 (92%)	-0.25	0 100 100	16, 66, 146, 166	0
All	All	947/1024 (92%)	-0.26	0 100 100	15, 65, 131, 174	0

There are no RSRZ outliers to report.

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.