



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:30 PM UTC

PDB ID : 6IW2 / pdb_00006iw2
Title : Crystal structure of 5A ScFv in complex with YFV-17D sE in prefusion state
Authors : Lu, X.S.; Xiao, H.X.; Li, S.H.; Pang, X.F.
Deposited on : 2018-12-04
Resolution : 2.90 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

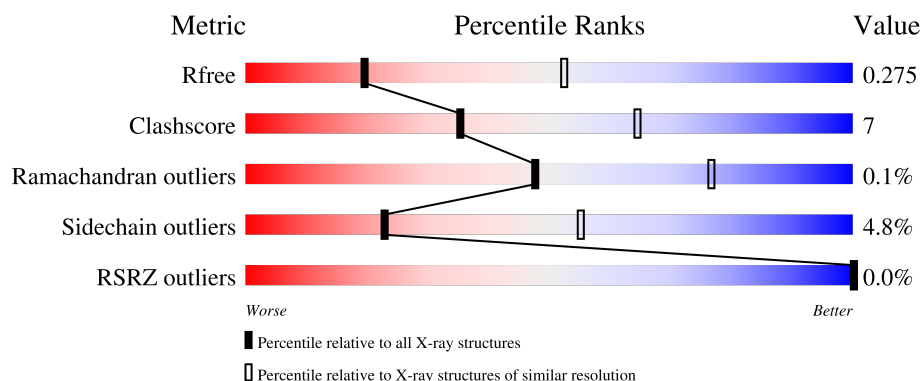
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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.



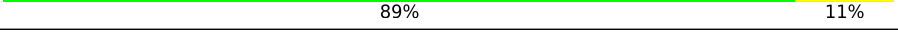
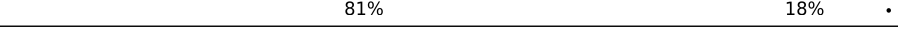
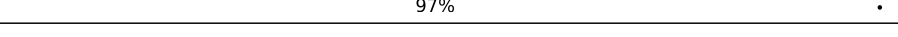
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	395	 77% 18% ..
1	D	395	 74% 21% ..
1	G	395	 77% 19% ...
1	J	395	 79% 17% ..
1	M	395	 77% 18% ..

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Mol	Chain	Length	Quality of chain
1	P	395	 77%19% . .
2	B	120	 76%23% .
2	E	120	 68%32% .
2	H	120	 76%22% .
2	K	120	 78%21% .
2	N	120	 70%28% .
2	Q	120	 79%19% .
3	C	107	 85%15%
3	F	107	 89%11%
3	I	107	 82%16% .
3	L	107	 81%18% .
3	O	107	 84%15% .
3	R	107	 97% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 28516 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 Envelope protein E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	S	0	0	0
			2965	1863	514	569	19			
1	D	388	Total	C	N	O	S	0	1	0
			2986	1877	518	572	19			
1	G	388	Total	C	N	O	S	0	0	0
			2979	1872	516	572	19			
1	J	387	Total	C	N	O	S	0	1	0
			2983	1877	516	571	19			
1	M	387	Total	C	N	O	S	0	0	0
			2972	1868	515	570	19			
1	P	387	Total	C	N	O	S	0	0	0
			2972	1868	515	570	19			

- Molecule 2 is a protein called Heavy chain of monoclonal antibody 5A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	120	Total	C	N	O	S	0	0	0
			954	606	158	187	3			
2	E	120	Total	C	N	O	S	0	0	0
			954	606	158	187	3			
2	H	120	Total	C	N	O	S	0	0	0
			954	606	158	187	3			
2	K	120	Total	C	N	O	S	0	0	0
			954	606	158	187	3			
2	N	120	Total	C	N	O	S	0	1	0
			960	610	158	189	3			
2	Q	120	Total	C	N	O	S	0	0	0
			954	606	158	187	3			

- Molecule 3 is a protein called Light chain of monoclonal antibody 5A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	107	Total	C	N	O	S	0	0	0
			823	523	134	163	3			
3	F	107	Total	C	N	O	S	0	0	0
			823	523	134	163	3			
3	I	107	Total	C	N	O	S	0	0	0
			823	523	134	163	3			
3	L	106	Total	C	N	O	S	0	0	0
			814	518	132	161	3			
3	O	107	Total	C	N	O	S	0	0	0
			823	523	134	163	3			
3	R	107	Total	C	N	O	S	0	0	0
			823	523	134	163	3			

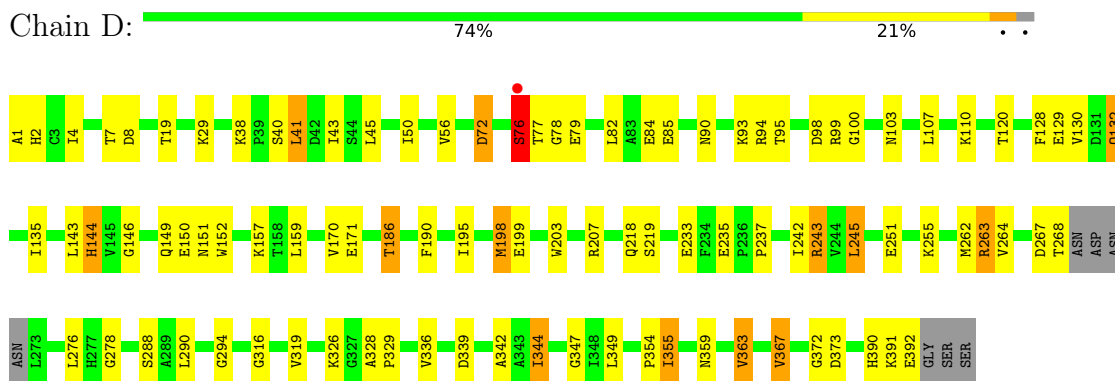
3 Residue-property plots [i](#)

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.

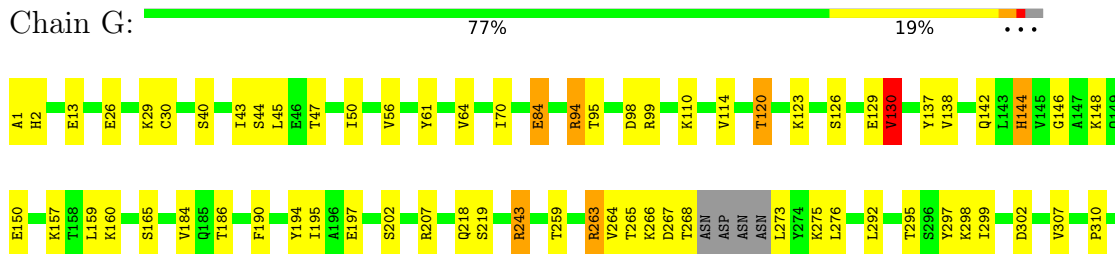
• Molecule 1: Envelope protein E



• Molecule 1: Envelope protein E



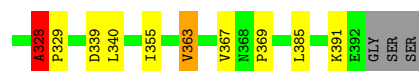
• Molecule 1: Envelope protein E





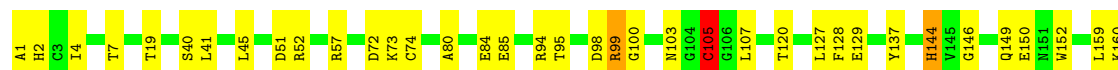
• Molecule 1: Envelope protein E

Chain J: 79% 17% ..



• Molecule 1: Envelope protein E

Chain M: 77% 18% ..



• Molecule 1: Envelope protein E

Chain P: 77% 19% ..

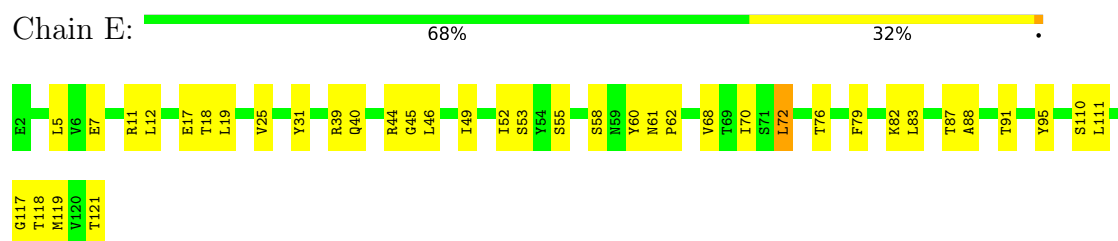


• Molecule 2: Heavy chain of monoclonal antibody 5A

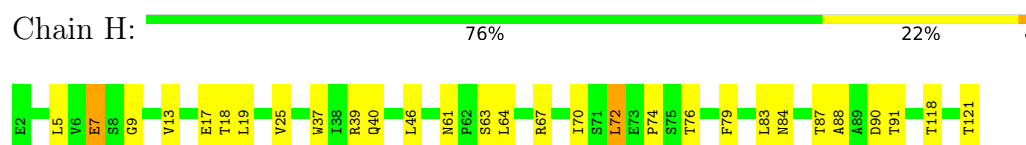
Chain B: 76% 23% .



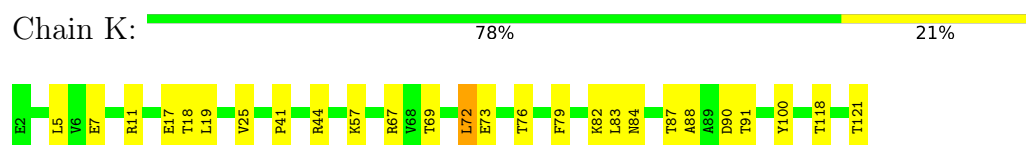
- Molecule 2: Heavy chain of monoclonal antibody 5A



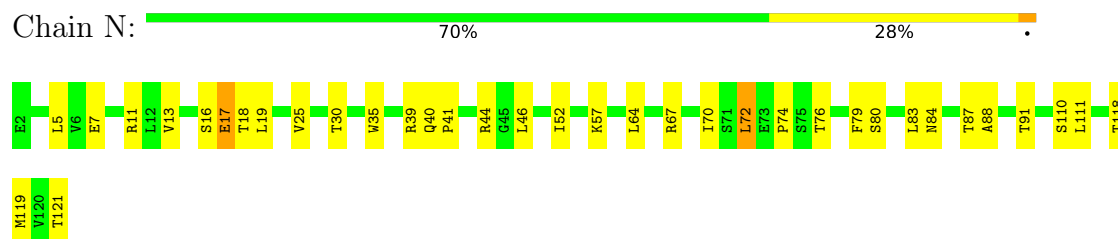
- Molecule 2: Heavy chain of monoclonal antibody 5A



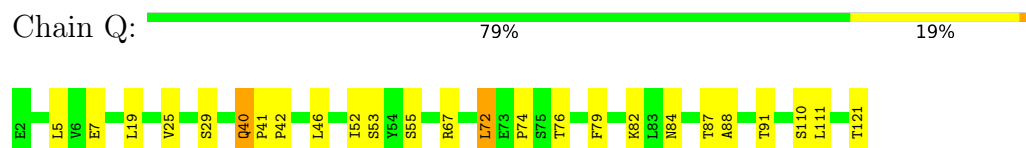
- Molecule 2: Heavy chain of monoclonal antibody 5A



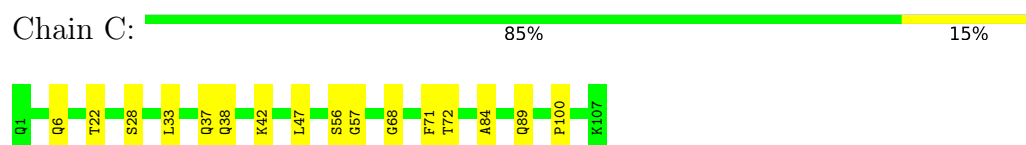
- Molecule 2: Heavy chain of monoclonal antibody 5A



- Molecule 2: Heavy chain of monoclonal antibody 5A



- Molecule 3: Light chain of monoclonal antibody 5A



- Molecule 3: Light chain of monoclonal antibody 5A

Chain F:  89% 11%



- Molecule 3: Light chain of monoclonal antibody 5A

Chain I:  82% 16%



- Molecule 3: Light chain of monoclonal antibody 5A

Chain L:  81% 18%

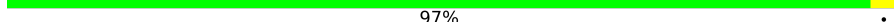


- Molecule 3: Light chain of monoclonal antibody 5A

Chain O:  84% 15%



- Molecule 3: Light chain of monoclonal antibody 5A

Chain R:  97%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	95.97Å 99.24Å 123.10Å 96.39° 94.90° 100.36°	Depositor
Resolution (Å)	48.70 – 2.90 48.70 – 2.90	Depositor EDS
% Data completeness (in resolution range)	85.2 (48.70-2.90) 78.1 (48.70-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.237 , 0.272 0.240 , 0.275	Depositor DCC
R_{free} test set	4170 reflections (4.23%)	wwPDB-VP
Wilson B-factor (Å ²)	50.9	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 22.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.106 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	28516	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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

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	0.33	0/3023	0.74	2/4098 (0.0%)
1	D	0.43	1/3049 (0.0%)	0.84	5/4135 (0.1%)
1	G	0.38	0/3038	0.83	4/4120 (0.1%)
1	J	0.34	0/3043	0.81	4/4126 (0.1%)
1	M	0.36	1/3031 (0.0%)	0.75	0/4110
1	P	0.33	0/3031	0.83	2/4110 (0.0%)
2	B	0.30	0/982	0.84	4/1342 (0.3%)
2	E	0.39	0/982	0.84	1/1342 (0.1%)
2	H	0.31	0/982	0.80	2/1342 (0.1%)
2	K	0.31	0/982	0.84	2/1342 (0.1%)
2	N	0.31	0/991	0.80	0/1355
2	Q	0.29	0/982	0.81	2/1342 (0.1%)
3	C	0.28	0/843	0.71	0/1144
3	F	0.28	0/843	0.70	0/1144
3	I	0.30	0/843	0.74	0/1144
3	L	0.29	0/834	0.69	0/1132
3	O	0.38	0/843	0.78	0/1144
3	R	0.27	0/843	0.74	2/1144 (0.2%)
All	All	0.34	2/29165 (0.0%)	0.79	30/39616 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	199	GLU	CA-C	-10.37	1.45	1.52
1	M	105	CYS	C-O	-5.26	1.17	1.23

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	165	SER	N-CA-C	-7.87	98.23	110.42
2	K	73	GLU	CA-C-N	7.59	127.24	119.19
2	K	73	GLU	C-N-CA	7.59	127.24	119.19
1	P	102	GLY	N-CA-C	-6.61	106.51	113.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	40	GLN	CA-C-N	6.58	124.47	119.66
2	B	40	GLN	C-N-CA	6.58	124.47	119.66
1	D	186	THR	N-CA-C	6.52	118.18	111.14
2	E	119	MET	N-CA-C	6.24	118.33	108.67
1	A	105	CYS	N-CA-C	-6.21	99.69	109.50
2	Q	40	GLN	CA-C-N	6.00	124.04	119.66
2	Q	40	GLN	C-N-CA	6.00	124.04	119.66
1	J	222	GLY	N-CA-C	-5.56	100.00	113.18
1	P	165	SER	N-CA-C	-5.54	102.26	110.46
1	J	328	ALA	CA-C-N	-5.49	112.98	119.84
1	J	328	ALA	C-N-CA	-5.49	112.98	119.84
2	B	9	GLY	CA-C-N	5.42	126.61	119.84
2	B	9	GLY	C-N-CA	5.42	126.61	119.84
1	D	132	GLN	CB-CG-CD	-5.36	103.50	112.60
1	D	76	SER	CB-CA-C	-5.32	110.00	117.23
3	R	58	VAL	CA-C-N	5.30	125.30	119.90
3	R	58	VAL	C-N-CA	5.30	125.30	119.90
1	G	130	VAL	N-CA-C	5.26	115.43	107.80
1	A	189	ASP	N-CA-C	-5.24	98.29	107.73
1	D	78	GLY	N-CA-C	5.21	125.53	113.18
1	J	166	GLY	N-CA-C	-5.17	105.20	112.60
1	D	72	ASP	N-CA-C	5.12	116.55	109.54
1	G	328	ALA	CA-C-N	-5.11	113.45	119.84
1	G	328	ALA	C-N-CA	-5.11	113.45	119.84
2	H	9	GLY	CA-C-N	5.08	126.20	119.84
2	H	9	GLY	C-N-CA	5.08	126.20	119.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2965	0	2915	48	0
1	D	2986	0	2938	61	0
1	G	2979	0	2931	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	2983	0	2932	39	0
1	M	2972	0	2925	45	0
1	P	2972	0	2924	44	0
2	B	954	0	907	13	0
2	E	954	0	907	20	0
2	H	954	0	907	16	0
2	K	954	0	907	12	0
2	N	960	0	913	19	0
2	Q	954	0	907	13	0
3	C	823	0	807	8	0
3	F	823	0	807	5	0
3	I	823	0	807	13	0
3	L	814	0	796	10	0
3	O	823	0	807	9	0
3	R	823	0	807	2	0
All	All	28516	0	27844	414	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 7.

All (414) 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:M:74:CYS:CB	1:M:105:CYS:SG	2.04	1.45
1:M:74:CYS:SG	1:M:105:CYS:SG	1.43	1.43
1:D:186:THR:HG21	1:D:190:PHE:CE2	2.04	0.93
1:D:186:THR:HG21	1:D:190:PHE:HE2	1.34	0.91
3:I:24:ARG:HH11	3:I:69:THR:HG22	1.36	0.88
1:M:146:GLY:HA3	1:M:363:VAL:HG23	1.57	0.87
1:M:74:CYS:HB3	1:M:105:CYS:SG	2.12	0.87
1:J:146:GLY:HA3	1:J:363:VAL:HG23	1.57	0.85
1:M:74:CYS:CA	1:M:105:CYS:SG	2.66	0.83
1:P:146:GLY:HA3	1:P:363:VAL:HG23	1.60	0.83
1:P:79:GLU:HG3	1:P:94:ARG:HH12	1.45	0.81
1:D:146:GLY:HA3	1:D:363:VAL:HG23	1.62	0.81
1:A:129:GLU:HG2	1:A:207:ARG:HH11	1.45	0.80
1:G:146:GLY:HA3	1:G:363:VAL:HG23	1.63	0.80
2:E:11:ARG:HH12	2:E:118:THR:HB	1.50	0.77
3:O:24:ARG:HH11	3:O:69:THR:HG22	1.51	0.76
1:D:373:ASP:OD1	1:D:390:HIS:ND1	2.19	0.74
2:K:72:LEU:HD23	2:K:79:PHE:HB3	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:80:ALA:O	1:M:94:ARG:NH2	2.21	0.72
1:P:160:LYS:O	1:P:168:GLN:NE2	2.21	0.72
1:J:201:GLU:OE1	1:J:263:ARG:NH2	2.22	0.72
1:A:146:GLY:HA3	1:A:363:VAL:HG23	1.73	0.71
2:E:91:THR:HG23	2:E:121:THR:HA	1.72	0.70
2:E:11:ARG:NH1	2:E:118:THR:HB	2.06	0.70
2:K:41:PRO:HB2	2:K:44:ARG:HD3	1.73	0.69
1:M:295:THR:O	1:M:331:ARG:NH2	2.25	0.69
1:D:326:LYS:O	1:D:359:ASN:ND2	2.26	0.69
1:M:74:CYS:HA	1:M:105:CYS:SG	2.32	0.69
1:A:292:LEU:HD21	1:A:353:ASN:HB3	1.73	0.69
2:E:44:ARG:HG2	2:E:45:GLY:H	1.57	0.69
1:A:50:ILE:HD12	1:A:195:ILE:HD11	1.75	0.67
1:P:131:ASP:OD2	1:P:134:LYS:NZ	2.26	0.67
1:G:84:GLU:OE2	3:I:56:SER:OG	2.11	0.67
2:Q:5:LEU:HD22	2:Q:25:VAL:HG22	1.77	0.67
1:D:235:GLU:OE1	1:D:243:ARG:NH1	2.28	0.66
1:J:85:GLU:OE2	1:J:94:ARG:NH1	2.26	0.66
1:P:50:ILE:HD12	1:P:195:ILE:HD11	1.76	0.66
1:M:202:SER:HB2	1:M:264:VAL:HB	1.77	0.65
2:H:72:LEU:HD23	2:H:79:PHE:HB3	1.76	0.65
2:H:61:ASN:ND2	2:H:63:SER:OG	2.30	0.65
1:M:332:ILE:HB	1:M:354:PRO:HB2	1.79	0.65
1:G:194:TYR:CZ	1:G:207:ARG:HD3	2.31	0.64
1:J:132:GLN:HE21	1:J:186:THR:HG21	1.60	0.64
1:P:286:LYS:NZ	1:P:288:SER:OG	2.30	0.64
2:B:72:LEU:HD23	2:B:79:PHE:HB3	1.80	0.64
1:D:198:MET:HG3	1:D:203:TRP:HZ3	1.61	0.64
1:M:73:LYS:O	1:M:99:ARG:NH1	2.31	0.64
1:D:40:SER:HB2	1:D:144:HIS:HB2	1.81	0.63
1:G:40:SER:HB2	1:G:144:HIS:HB2	1.80	0.63
1:G:267:ASP:OD1	1:G:268:THR:N	2.31	0.63
1:A:286:LYS:NZ	1:A:288:SER:OG	2.33	0.62
1:D:190:PHE:H	1:D:190:PHE:HD2	1.45	0.62
1:D:99:ARG:NH2	1:D:103:ASN:O	2.34	0.61
1:J:89:ASP:OD2	1:J:89:ASP:N	2.28	0.61
1:M:57:ARG:HG3	1:M:127:LEU:HD12	1.83	0.61
1:P:128:PHE:HB2	1:P:195:ILE:HB	1.83	0.61
2:B:17:GLU:HG2	2:B:18:THR:H	1.65	0.61
2:E:5:LEU:HD22	2:E:25:VAL:HG22	1.81	0.61
2:B:5:LEU:HD22	2:B:25:VAL:HG22	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:218:GLN:HG2	1:G:219:SER:H	1.66	0.60
2:N:91:THR:HG23	2:N:121:THR:HA	1.84	0.59
1:P:198:MET:CE	1:P:251:GLU:HG3	2.32	0.59
2:E:72:LEU:HD23	2:E:79:PHE:HB3	1.83	0.59
1:G:202:SER:HB2	1:G:264:VAL:HB	1.84	0.59
1:A:74:CYS:HB2	1:A:105:CYS:SG	2.13	0.59
1:A:74:CYS:SG	1:A:75:PRO:HD2	2.42	0.59
2:E:40:GLN:HB2	2:E:46:LEU:HD23	1.84	0.59
1:G:298:LYS:HZ1	1:G:328:ALA:HB3	1.68	0.58
2:N:5:LEU:HD22	2:N:25:VAL:HG22	1.85	0.58
1:P:266:LYS:HB3	1:P:274:TYR:HA	1.84	0.58
1:J:305[B]:PHE:CZ	1:J:323:LYS:HD2	2.38	0.58
1:M:129:GLU:HG3	1:M:207:ARG:HH12	1.68	0.58
1:P:266:LYS:O	1:P:267:ASP:HB2	2.03	0.58
1:P:56:VAL:HG21	1:P:129:GLU:HG3	1.86	0.58
3:O:5:THR:OG1	3:O:24:ARG:HB3	2.04	0.57
1:M:128:PHE:HB2	1:M:195:ILE:HB	1.86	0.57
1:G:298:LYS:NZ	1:G:328:ALA:HB3	2.19	0.57
1:J:99:ARG:HA	1:J:103:ASN:HD21	1.68	0.57
2:K:91:THR:HG23	2:K:121:THR:HA	1.86	0.57
2:Q:72:LEU:HD23	2:Q:79:PHE:HB3	1.85	0.57
2:E:19:LEU:O	2:E:82:LYS:HA	2.05	0.57
1:A:264:VAL:HG22	1:A:276:LEU:HD13	1.86	0.57
2:H:13:VAL:HG21	2:H:19:LEU:HD13	1.87	0.56
1:D:135:ILE:HD11	1:D:190:PHE:HZ	1.70	0.56
1:D:342:ALA:HB1	1:D:344:ILE:HG13	1.86	0.56
1:G:186:THR:HG21	1:G:190:PHE:CE2	2.40	0.56
2:N:13:VAL:HG21	2:N:19:LEU:HD13	1.88	0.56
1:P:186:THR:HG22	1:P:188:VAL:H	1.70	0.56
1:D:316:GLY:O	1:D:391:LYS:NZ	2.26	0.56
2:H:67:ARG:NH1	2:H:90:ASP:OD2	2.28	0.56
1:J:179:THR:HB	1:J:286:LYS:HB3	1.88	0.56
1:P:72:ASP:OD1	2:Q:29:SER:OG	2.23	0.56
1:D:50:ILE:HD12	1:D:195:ILE:HD11	1.88	0.56
1:J:79:GLU:HG3	1:J:94:ARG:HH21	1.71	0.56
1:D:267:ASP:OD1	1:D:268:THR:N	2.39	0.56
2:K:17:GLU:HG2	2:K:18:THR:H	1.70	0.56
1:D:128:PHE:HB2	1:D:195:ILE:HB	1.86	0.55
2:N:72:LEU:HD13	2:N:74:PRO:HD3	1.87	0.55
2:K:5:LEU:HD22	2:K:25:VAL:HG22	1.88	0.55
1:D:372:GLY:HA2	1:D:392:GLU:OE2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:264:VAL:HG22	1:M:276:LEU:HD13	1.89	0.55
1:J:79:GLU:HG3	1:J:94:ARG:NH2	2.22	0.55
1:G:264:VAL:HG13	1:G:275:LYS:O	2.06	0.55
2:N:67:ARG:HD2	2:N:84:ASN:O	2.07	0.55
2:B:91:THR:HG23	2:B:121:THR:HA	1.89	0.55
1:J:202:SER:HB2	1:J:264:VAL:HB	1.87	0.54
3:I:18:ARG:HG3	3:I:76:SER:HA	1.87	0.54
1:D:349:LEU:HD21	1:D:354:PRO:HD3	1.88	0.54
1:J:218:GLN:HG2	1:J:219:SER:H	1.73	0.54
1:A:160:LYS:O	1:A:168:GLN:NE2	2.38	0.54
2:H:5:LEU:HD22	2:H:25:VAL:HG22	1.88	0.54
3:I:24:ARG:HH12	3:I:70:GLU:HG2	1.71	0.54
1:M:85:GLU:OE2	1:M:94:ARG:NE	2.38	0.54
2:H:91:THR:HG23	2:H:121:THR:HA	1.90	0.54
1:J:41:LEU:HD22	1:J:43:ILE:HG12	1.90	0.53
1:A:56:VAL:HG21	1:A:129:GLU:HG3	1.90	0.53
1:D:294:GLY:HA3	1:D:355:ILE:HD11	1.91	0.53
2:E:11:ARG:HB3	2:E:12:LEU:HD12	1.91	0.53
1:J:80:ALA:O	1:J:94:ARG:NH2	2.39	0.52
1:P:137:TYR:CE1	1:P:184:VAL:HB	2.44	0.52
1:D:218:GLN:HG2	1:D:219:SER:H	1.73	0.52
1:G:138:VAL:HG22	1:G:160:LYS:HD3	1.92	0.52
1:G:148:LYS:HD2	1:G:362:GLU:HB2	1.92	0.52
3:I:5:THR:OG1	3:I:24:ARG:HB3	2.10	0.52
1:J:174:GLY:O	1:J:293:LYS:HB2	2.10	0.52
1:G:94:ARG:HD2	1:G:114:VAL:HG22	1.90	0.52
1:D:149:GLN:HA	1:D:152:TRP:CD2	2.44	0.52
1:G:61:TYR:CE2	1:G:123:LYS:HE2	2.45	0.52
3:L:37:GLN:HE21	3:L:47:LEU:HD11	1.74	0.52
1:G:186:THR:HG21	1:G:190:PHE:CZ	2.44	0.52
1:J:304:MET:HE2	1:J:324:VAL:HG22	1.90	0.52
1:J:8:ASP:OD2	1:J:29:LYS:HE2	2.10	0.52
1:A:192:ASN:HA	1:A:207:ARG:HD2	1.91	0.51
1:D:130:VAL:HG22	1:D:195:ILE:HG13	1.92	0.51
2:Q:91:THR:HG23	2:Q:121:THR:HA	1.91	0.51
1:M:7:THR:HG21	1:P:98:ASP:HB3	1.92	0.51
1:M:218:GLN:HG2	1:M:219:SER:H	1.76	0.51
2:B:13:VAL:HG21	2:B:19:LEU:HD13	1.93	0.51
1:D:264:VAL:HG22	1:D:276:LEU:HD13	1.92	0.51
2:K:69:THR:HB	2:K:82:LYS:HB2	1.91	0.51
2:N:11:ARG:CZ	2:N:118:THR:HB	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:349:LEU:HD12	1:D:367:VAL:HG13	1.92	0.51
1:J:50:ILE:HD12	1:J:195:ILE:HD11	1.92	0.51
1:M:266:LYS:HD3	1:M:274:TYR:CZ	2.46	0.51
1:G:56:VAL:CG2	1:G:129:GLU:HB2	2.41	0.51
1:J:339:ASP:OD1	1:J:340:LEU:N	2.44	0.50
2:Q:72:LEU:HD13	2:Q:74:PRO:HD3	1.92	0.50
1:J:128:PHE:HB2	1:J:195:ILE:HB	1.92	0.50
1:G:56:VAL:HG21	1:G:129:GLU:HB2	1.93	0.50
3:I:24:ARG:NH1	3:I:69:THR:HG22	2.15	0.50
1:A:7:THR:HG21	1:D:98:ASP:HB3	1.94	0.50
1:A:57:ARG:HB3	1:A:127:LEU:HB2	1.93	0.50
1:J:328:ALA:HB1	1:J:329:PRO:HD2	1.94	0.50
2:N:41:PRO:HB2	2:N:44:ARG:HD3	1.93	0.50
1:G:297:TYR:N	1:G:331:ARG:HH22	2.10	0.50
1:M:160:LYS:O	1:M:168:GLN:NE2	2.37	0.50
3:C:33:LEU:HD22	3:C:71:PHE:CG	2.47	0.50
2:N:40:GLN:HB2	2:N:46:LEU:HD23	1.94	0.50
1:A:89:ASP:OD2	1:A:89:ASP:N	2.41	0.49
1:D:41:LEU:HD22	1:D:43:ILE:HG12	1.95	0.49
2:Q:53:SER:OG	2:Q:55:SER:OG	2.28	0.49
1:M:149:GLN:HA	1:M:152:TRP:CE2	2.48	0.49
1:D:38:LYS:NZ	1:D:288:SER:HA	2.27	0.49
1:D:198:MET:HE1	1:D:251:GLU:HG3	1.94	0.49
1:D:8:ASP:OD2	1:D:29:LYS:HE2	2.13	0.49
1:G:324:VAL:HG21	1:G:356:ALA:HB2	1.94	0.49
1:A:16:HIS:HA	1:A:36:PRO:HG2	1.95	0.49
1:G:266:LYS:O	1:G:266:LYS:HG3	2.12	0.49
1:P:100:GLY:HA2	1:P:107:LEU:O	2.13	0.49
1:P:185:GLN:HG3	1:P:280:HIS:CE1	2.47	0.49
1:D:130:VAL:HG12	1:D:190:PHE:CE1	2.48	0.49
1:D:190:PHE:N	1:D:190:PHE:CD2	2.79	0.49
1:P:328:ALA:HB1	1:P:329:PRO:HD2	1.95	0.49
1:J:201:GLU:HB3	1:J:263:ARG:HH22	1.78	0.48
2:N:17:GLU:HG3	2:N:18:THR:H	1.76	0.48
1:P:110:LYS:HA	1:P:110:LYS:HD3	1.53	0.48
1:J:4:ILE:HD13	1:J:319:VAL:HG11	1.95	0.48
1:P:8:ASP:OD2	1:P:29:LYS:HE2	2.13	0.48
1:A:256:THR:O	1:A:259:THR:OG1	2.31	0.48
1:G:50:ILE:HD12	1:G:195:ILE:HD11	1.95	0.48
2:B:67:ARG:HD2	2:B:84:ASN:O	2.13	0.48
1:D:339:ASP:OD1	1:D:342:ALA:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:50:ILE:HD13	1:G:130:VAL:HG13	1.93	0.48
1:J:38:LYS:NZ	1:J:288:SER:HA	2.27	0.48
1:A:62:ASN:HD22	1:A:249:ASN:ND2	2.12	0.48
1:G:307:VAL:N	1:G:321:GLN:O	2.46	0.48
1:G:64:VAL:HG23	1:G:120:THR:HG23	1.94	0.48
1:A:327:GLY:O	1:A:359:ASN:ND2	2.46	0.48
1:D:72:ASP:O	1:D:99:ARG:NH1	2.47	0.48
1:M:237:PRO:HB3	1:M:242:ILE:HG12	1.96	0.48
2:N:72:LEU:HD23	2:N:79:PHE:HB3	1.95	0.48
1:J:40:SER:HB2	1:J:144:HIS:HB2	1.96	0.48
1:J:99:ARG:HA	1:J:103:ASN:ND2	2.29	0.48
1:P:297:TYR:HB3	1:P:330:CYS:HA	1.96	0.48
1:D:186:THR:HG21	1:D:190:PHE:CZ	2.46	0.48
1:D:149:GLN:HA	1:D:152:TRP:CE2	2.49	0.47
3:O:37:GLN:HE21	3:O:47:LEU:HD11	1.79	0.47
3:L:56:SER:HA	3:L:57:GLY:HA2	1.56	0.47
2:H:17:GLU:CD	2:H:18:THR:H	2.21	0.47
1:P:149:GLN:HA	1:P:152:TRP:CD2	2.49	0.47
1:A:56:VAL:HG21	1:A:129:GLU:CG	2.44	0.47
2:N:52:ILE:HD13	2:N:72:LEU:HB2	1.96	0.47
1:P:294:GLY:HA3	1:P:355:ILE:HD11	1.95	0.47
1:A:189:ASP:O	1:A:192:ASN:N	2.34	0.47
1:M:100:GLY:HA2	1:M:107:LEU:O	2.14	0.47
2:N:30:THR:HA	2:N:35:TRP:CZ2	2.50	0.47
2:Q:40:GLN:HB2	2:Q:46:LEU:HD23	1.96	0.47
1:A:202:SER:HB2	1:A:264:VAL:HB	1.96	0.47
1:P:298:LYS:NZ	1:P:328:ALA:HB3	2.30	0.47
1:A:324:VAL:O	1:A:360:ASP:N	2.48	0.47
1:P:118:LYS:NZ	1:P:120:THR:HB	2.30	0.46
1:G:299:ILE:HD13	1:G:380:ARG:HH21	1.79	0.46
1:M:137:TYR:CE2	1:M:184:VAL:HB	2.50	0.46
1:D:198:MET:HG3	1:D:203:TRP:CZ3	2.46	0.46
3:L:47:LEU:HA	3:L:58:VAL:HG21	1.97	0.46
1:M:107:LEU:HD23	1:M:107:LEU:HA	1.78	0.46
1:M:174:GLY:O	1:M:293:LYS:HB2	2.15	0.46
1:A:84:GLU:OE2	3:C:56:SER:OG	2.30	0.46
3:I:10:THR:HG23	3:I:103:LYS:HB3	1.97	0.46
3:L:35:TRP:HB2	3:L:48:ILE:HB	1.98	0.46
2:E:68:VAL:HG22	2:E:83:LEU:HD13	1.96	0.46
2:E:87:THR:OG1	2:E:88:ALA:N	2.49	0.46
1:J:14:GLY:N	1:J:34:MET:O	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:264:VAL:HG22	1:J:276:LEU:HD13	1.98	0.46
1:P:64:VAL:HG23	1:P:120:THR:HG23	1.98	0.46
1:D:132:GLN:HA	1:D:190:PHE:CE1	2.51	0.46
1:M:159:LEU:HD21	1:M:170:VAL:HG22	1.98	0.46
3:C:37:GLN:HB2	3:C:47:LEU:HD11	1.98	0.46
1:A:64:VAL:HG23	1:A:120:THR:HG23	1.97	0.46
1:G:61:TYR:HE2	1:G:123:LYS:HE2	1.81	0.46
1:P:1:ALA:HB1	1:P:142:GLN:HB3	1.97	0.46
1:P:218:GLN:HG2	1:P:219:SER:H	1.80	0.46
1:G:328:ALA:HB1	1:G:329:PRO:HD2	1.98	0.45
1:J:64:VAL:HG23	1:J:120:THR:HG23	1.99	0.45
3:O:33:LEU:HD22	3:O:71:PHE:CG	2.50	0.45
2:Q:87:THR:OG1	2:Q:88:ALA:N	2.49	0.45
1:A:1:ALA:HB1	1:A:142:GLN:HB3	1.98	0.45
1:D:103:ASN:HA	2:E:31:TYR:CD2	2.51	0.45
2:H:17:GLU:CG	2:H:18:THR:H	2.29	0.45
1:M:40:SER:HB2	1:M:144:HIS:HB2	1.99	0.45
1:M:51:ASP:OD2	1:M:52:ARG:NE	2.48	0.45
3:O:4:MET:HA	3:O:24:ARG:O	2.17	0.45
1:A:74:CYS:O	1:A:77:THR:HG22	2.17	0.45
1:A:143:LEU:HD21	1:A:290:LEU:HD21	1.99	0.45
1:D:328:ALA:HB1	1:D:329:PRO:HD2	1.98	0.45
1:G:1:ALA:HA	1:G:2:HIS:HA	1.68	0.45
2:H:19:LEU:HB3	2:H:83:LEU:HB3	1.97	0.45
1:M:299:ILE:HD13	1:M:380:ARG:HE	1.82	0.45
1:M:339:ASP:OD2	1:M:342:ALA:N	2.38	0.45
1:P:84:GLU:H	1:P:84:GLU:HG2	1.49	0.45
1:D:56:VAL:CG2	1:D:129:GLU:HB2	2.46	0.45
2:E:17:GLU:HG2	2:E:18:THR:H	1.81	0.45
2:E:39:ARG:HB3	2:E:49:ILE:HD11	1.99	0.45
1:G:137:TYR:CE1	1:G:184:VAL:HB	2.52	0.45
1:M:275:LYS:H	1:M:275:LYS:HG2	1.48	0.45
1:A:174:GLY:O	1:A:293:LYS:HB2	2.17	0.45
2:Q:67:ARG:HD2	2:Q:84:ASN:O	2.17	0.45
2:Q:110:SER:OG	2:Q:111:LEU:N	2.49	0.45
1:J:294:GLY:HA3	1:J:355:ILE:HD11	1.98	0.45
1:M:159:LEU:HD22	1:M:180:LEU:HD12	1.98	0.45
1:D:143:LEU:HD21	1:D:290:LEU:HD21	1.99	0.44
3:L:37:GLN:OE1	3:L:39:LYS:HE3	2.17	0.44
1:A:38:LYS:NZ	1:A:288:SER:HA	2.33	0.44
1:D:82:LEU:O	1:D:85:GLU:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:297:TYR:O	1:G:331:ARG:NH1	2.51	0.44
1:G:375:TYR:CE1	1:G:388:GLN:HG2	2.52	0.44
2:H:67:ARG:HD2	2:H:84:ASN:O	2.17	0.44
3:L:21:ILE:HD11	3:L:104:LEU:HD12	1.98	0.44
1:P:4:ILE:HD12	1:P:319:VAL:HG11	1.99	0.44
1:P:38:LYS:HE2	1:P:290:LEU:O	2.18	0.44
1:P:143:LEU:HD21	1:P:290:LEU:HD21	1.99	0.44
1:P:237:PRO:HB3	1:P:242:ILE:HG12	1.99	0.44
3:R:56:SER:HA	3:R:57:GLY:HA2	1.54	0.44
3:I:33:LEU:HD22	3:I:71:PHE:CG	2.53	0.44
1:M:294:GLY:HA3	1:M:355:ILE:HD11	1.99	0.44
1:D:198:MET:CE	1:D:251:GLU:HG3	2.48	0.44
1:G:263:ARG:NH1	1:G:263:ARG:HB3	2.32	0.44
2:B:39:ARG:NH2	2:B:64:LEU:HD21	2.32	0.44
2:H:40:GLN:HB2	2:H:46:LEU:HD23	2.00	0.44
1:P:262:MET:HE3	1:P:278:GLY:HA3	2.00	0.44
2:B:39:ARG:HB3	2:B:49:ILE:HD11	1.99	0.44
3:I:56:SER:HA	3:I:57:GLY:HA2	1.56	0.44
1:M:262:MET:HE2	1:M:262:MET:HB3	1.94	0.44
1:G:243:ARG:HD3	1:G:243:ARG:C	2.43	0.44
1:G:338:ASP:OD1	1:G:338:ASP:N	2.48	0.44
1:J:89:ASP:OD1	1:J:118:LYS:HE3	2.18	0.44
3:L:10:THR:HG23	3:L:103:LYS:HB3	2.00	0.44
1:A:1:ALA:HA	1:A:2:HIS:HA	1.69	0.43
1:A:40:SER:HB2	1:A:144:HIS:HB2	1.99	0.43
1:A:80:ALA:O	1:A:94:ARG:NH2	2.45	0.43
3:O:28:SER:HA	3:O:68:GLY:O	2.18	0.43
1:A:149:GLN:HA	1:A:152:TRP:CE2	2.53	0.43
1:D:1:ALA:HA	1:D:2:HIS:HA	1.66	0.43
3:I:37:GLN:HB2	3:I:47:LEU:HD11	1.99	0.43
1:A:84:GLU:H	1:A:84:GLU:HG2	1.48	0.43
1:M:328:ALA:HB1	1:M:329:PRO:HD2	2.01	0.43
1:A:266:LYS:HD3	1:A:274:TYR:CZ	2.54	0.43
2:E:52:ILE:HG13	2:E:58:SER:HB3	1.99	0.43
2:K:87:THR:OG1	2:K:88:ALA:N	2.52	0.43
1:M:162:ASP:O	1:M:163:ALA:C	2.61	0.43
3:C:38:GLN:O	3:C:84:ALA:HB1	2.18	0.43
1:D:50:ILE:HD13	1:D:130:VAL:HG13	2.00	0.43
2:E:61:ASN:OD1	2:E:62:PRO:HD2	2.18	0.43
3:L:24:ARG:HG3	3:L:69:THR:HG22	2.00	0.43
1:M:4:ILE:HD13	1:M:319:VAL:HG11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:GLU:OE2	1:D:245:LEU:HD21	2.19	0.43
1:D:336:VAL:HB	1:D:347:GLY:HA3	2.01	0.43
3:O:56:SER:HA	3:O:57:GLY:HA2	1.59	0.43
2:Q:19:LEU:O	2:Q:82:LYS:HA	2.19	0.43
3:C:22:THR:HG22	3:C:72:THR:HG22	2.00	0.43
2:E:53:SER:OG	2:E:55:SER:OG	2.31	0.43
2:K:19:LEU:HB3	2:K:83:LEU:HB3	2.01	0.43
1:M:369:PRO:HG2	1:M:391:LYS:HD2	2.00	0.43
1:G:310:PRO:HD2	1:G:387:TYR:CD2	2.54	0.43
3:I:47:LEU:HA	3:I:58:VAL:HG21	2.00	0.43
1:J:132:GLN:HG3	1:J:190:PHE:HB3	2.00	0.43
1:P:50:ILE:HD13	1:P:130:VAL:HG13	2.01	0.43
1:P:118:LYS:HZ2	1:P:120:THR:HB	1.84	0.43
1:A:236:PRO:HA	1:A:237:PRO:HD3	1.84	0.42
3:I:38:GLN:O	3:I:84:ALA:HB1	2.19	0.42
2:K:67:ARG:NH1	2:K:90:ASP:OD2	2.48	0.42
2:N:52:ILE:HD12	2:N:70:ILE:O	2.19	0.42
1:P:84:GLU:OE2	3:R:56:SER:OG	2.29	0.42
1:D:237:PRO:HB3	1:D:242:ILE:HG12	2.01	0.42
1:M:98:ASP:HB3	1:P:7:THR:HG21	2.01	0.42
2:B:110:SER:OG	2:B:111:LEU:N	2.52	0.42
1:D:79:GLU:HG3	1:D:94:ARG:HH22	1.85	0.42
2:E:110:SER:OG	2:E:111:LEU:N	2.52	0.42
3:I:36:TYR:HE1	3:I:89:GLN:HE21	1.67	0.42
1:P:326:LYS:O	1:P:359:ASN:ND2	2.53	0.42
1:A:4:ILE:HD13	1:A:319:VAL:HG11	2.01	0.42
1:A:56:VAL:HG21	1:A:129:GLU:CD	2.44	0.42
1:G:1:ALA:HB1	1:G:142:GLN:HB3	2.00	0.42
2:Q:52:ILE:HD13	2:Q:72:LEU:HB2	2.02	0.42
1:A:95:THR:HG22	1:A:96:TYR:H	1.85	0.42
1:P:46:GLU:HG2	1:P:47:THR:HG23	2.01	0.42
1:P:179:THR:HB	1:P:286:LYS:HB3	2.01	0.42
1:D:198:MET:HE2	1:D:255:LYS:HE3	2.02	0.42
3:F:37:GLN:HE21	3:F:47:LEU:HD11	1.83	0.42
3:F:41:GLY:C	3:F:42:LYS:HD2	2.45	0.42
3:L:89:GLN:HB2	3:L:98:PHE:CD2	2.54	0.42
2:N:19:LEU:HB3	2:N:83:LEU:HB3	2.01	0.42
1:P:58:LYS:HB2	1:P:218:GLN:HB3	2.02	0.42
1:A:333:PRO:HG2	1:A:379:GLY:HA2	2.01	0.42
1:J:38:LYS:HZ3	1:J:288:SER:HA	1.83	0.42
3:L:28:SER:HA	3:L:68:GLY:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:56:SER:HA	3:C:57:GLY:HA2	1.55	0.42
1:D:129:GLU:HG3	1:D:207:ARG:NH2	2.35	0.42
2:B:72:LEU:HD13	2:B:74:PRO:HD3	2.01	0.41
1:D:76:SER:HB3	1:D:77:THR:H	1.54	0.41
1:G:47:THR:HG21	1:G:275:LYS:NZ	2.35	0.41
1:G:130:VAL:HG22	1:G:195:ILE:HG13	2.02	0.41
1:G:302:ASP:OD2	1:G:326:LYS:HB2	2.20	0.41
1:G:339:ASP:OD1	1:G:340:LEU:N	2.53	0.41
3:O:24:ARG:HH12	3:O:70:GLU:HG2	1.84	0.41
3:O:38:GLN:O	3:O:84:ALA:HB1	2.20	0.41
2:N:39:ARG:NH2	2:N:64:LEU:HD21	2.35	0.41
1:A:138:VAL:HA	1:A:159:LEU:O	2.20	0.41
1:A:198:MET:HE1	1:A:251:GLU:HG3	2.02	0.41
1:G:295:THR:C	1:G:331:ARG:NH2	2.78	0.41
2:E:60:TYR:HE2	2:E:70:ILE:HG13	1.85	0.41
3:F:56:SER:HA	3:F:57:GLY:HA2	1.54	0.41
1:G:297:TYR:N	1:G:331:ARG:NH2	2.69	0.41
1:J:304:MET:O	1:J:385:LEU:HD21	2.20	0.41
1:M:159:LEU:HD21	1:M:170:VAL:CG2	2.49	0.41
1:D:262:MET:HE3	1:D:278:GLY:HA3	2.02	0.41
2:K:67:ARG:HD2	2:K:84:ASN:O	2.20	0.41
1:G:292:LEU:HD12	1:G:292:LEU:HA	1.89	0.41
2:Q:41:PRO:HA	2:Q:42:PRO:HD3	1.96	0.41
1:D:4:ILE:HD13	1:D:319:VAL:HG11	2.03	0.41
1:D:263:ARG:HH11	1:D:263:ARG:HB3	1.85	0.41
1:G:30:CYS:HB2	1:G:44:SER:HB3	2.03	0.41
2:H:72:LEU:HD13	2:H:74:PRO:HD3	2.02	0.41
2:N:110:SER:OG	2:N:111:LEU:N	2.52	0.41
1:A:67:HIS:H	2:B:107:TYR:HE1	1.68	0.41
1:D:85:GLU:OE2	1:D:94:ARG:NH1	2.39	0.41
1:G:26:GLU:CD	1:G:29:LYS:HE3	2.46	0.41
1:J:227:GLU:HB3	1:J:230:HIS:CD2	2.56	0.41
1:M:266:LYS:O	1:M:266:LYS:HG3	2.20	0.41
2:B:87:THR:OG1	2:B:88:ALA:N	2.54	0.41
1:G:126:SER:HB2	1:G:197:GLU:HG2	2.02	0.41
1:G:307:VAL:HG21	1:G:362:GLU:HG2	2.03	0.41
2:H:7:GLU:HG2	2:H:118:THR:HG23	2.02	0.41
2:H:37:TRP:HD1	2:H:70:ILE:HD13	1.86	0.41
1:A:1:ALA:HB2	1:A:42:ASP:O	2.20	0.41
1:J:70:ILE:N	2:K:100:TYR:OH	2.53	0.41
1:J:369:PRO:HG2	1:J:391:LYS:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:338:ASP:OD1	1:P:338:ASP:N	2.41	0.41
3:C:6:GLN:HG3	3:C:100:PRO:HD2	2.02	0.40
1:D:84:GLU:HB3	1:D:90:ASN:ND2	2.37	0.40
1:D:100:GLY:HA2	1:D:107:LEU:O	2.21	0.40
1:J:1:ALA:HA	1:J:2:HIS:HA	1.70	0.40
1:A:98:ASP:HB3	1:D:7:THR:HG21	2.03	0.40
1:D:159:LEU:HD21	1:D:170:VAL:CG2	2.51	0.40
2:H:39:ARG:NH2	2:H:64:LEU:HD21	2.37	0.40
1:M:72:ASP:HB2	1:M:99:ARG:HH22	1.85	0.40
2:N:30:THR:HA	2:N:35:TRP:HZ2	1.86	0.40
1:A:41:LEU:HD22	1:A:43:ILE:HG12	2.03	0.40
1:M:1:ALA:HA	1:M:2:HIS:HA	1.70	0.40
1:M:137:TYR:CZ	1:M:161:PHE:HB2	2.56	0.40
1:A:139:ILE:HD11	1:A:281:VAL:HG11	2.04	0.40
2:B:37:TRP:HD1	2:B:70:ILE:HD13	1.86	0.40
3:C:28:SER:HA	3:C:68:GLY:O	2.22	0.40
3:F:28:SER:HA	3:F:68:GLY:O	2.20	0.40
3:F:33:LEU:HD22	3:F:71:PHE:CG	2.56	0.40
2:N:11:ARG:CD	2:N:119:MET:O	2.70	0.40
1:P:342:ALA:HB1	1:P:344:ILE:HG13	2.04	0.40
1:A:6:ILE:HD12	1:A:30:CYS:HB3	2.02	0.40
1:D:50:ILE:CD1	1:D:130:VAL:HG13	2.52	0.40
2:E:95:TYR:CE2	2:E:117:GLY:HA3	2.57	0.40
1:G:98:ASP:HB3	1:J:7:THR:HG21	2.03	0.40
2:H:87:THR:OG1	2:H:88:ALA:N	2.55	0.40
2:K:11:ARG:NH1	2:K:118:THR:HB	2.36	0.40
2:N:87:THR:OG1	2:N:88:ALA:N	2.55	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	380/395 (96%)	360 (95%)	20 (5%)	0	100	100
1	D	385/395 (98%)	358 (93%)	27 (7%)	0	100	100
1	G	384/395 (97%)	359 (94%)	24 (6%)	1 (0%)	36	65
1	J	384/395 (97%)	359 (94%)	24 (6%)	1 (0%)	36	65
1	M	383/395 (97%)	358 (94%)	23 (6%)	2 (0%)	24	54
1	P	383/395 (97%)	360 (94%)	23 (6%)	0	100	100
2	B	118/120 (98%)	113 (96%)	5 (4%)	0	100	100
2	E	118/120 (98%)	113 (96%)	5 (4%)	0	100	100
2	H	118/120 (98%)	113 (96%)	5 (4%)	0	100	100
2	K	118/120 (98%)	113 (96%)	5 (4%)	0	100	100
2	N	119/120 (99%)	116 (98%)	3 (2%)	0	100	100
2	Q	118/120 (98%)	113 (96%)	5 (4%)	0	100	100
3	C	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
3	F	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
3	I	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
3	L	104/107 (97%)	99 (95%)	5 (5%)	0	100	100
3	O	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
3	R	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
All	All	3637/3732 (98%)	3435 (94%)	198 (5%)	4 (0%)	48	77

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	327	GLY
1	M	328	ALA
1	J	328	ALA
1	G	328	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	322/331 (97%)	304 (94%)	18 (6%)	19	50
1	D	325/331 (98%)	304 (94%)	21 (6%)	15	44
1	G	324/331 (98%)	301 (93%)	23 (7%)	13	40
1	J	324/331 (98%)	306 (94%)	18 (6%)	19	50
1	M	323/331 (98%)	303 (94%)	20 (6%)	16	46
1	P	323/331 (98%)	308 (95%)	15 (5%)	24	57
2	B	107/107 (100%)	102 (95%)	5 (5%)	23	56
2	E	107/107 (100%)	104 (97%)	3 (3%)	38	72
2	H	107/107 (100%)	104 (97%)	3 (3%)	38	72
2	K	107/107 (100%)	103 (96%)	4 (4%)	30	64
2	N	108/107 (101%)	101 (94%)	7 (6%)	15	44
2	Q	107/107 (100%)	104 (97%)	3 (3%)	38	72
3	C	92/92 (100%)	90 (98%)	2 (2%)	45	77
3	F	92/92 (100%)	90 (98%)	2 (2%)	45	77
3	I	92/92 (100%)	90 (98%)	2 (2%)	45	77
3	L	91/92 (99%)	90 (99%)	1 (1%)	65	88
3	O	92/92 (100%)	89 (97%)	3 (3%)	33	67
3	R	92/92 (100%)	92 (100%)	0	100	100
All	All	3135/3180 (99%)	2985 (95%)	150 (5%)	23	55

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	THR
1	A	41	LEU
1	A	45	LEU
1	A	74	CYS
1	A	77	THR
1	A	84	GLU
1	A	87	GLU
1	A	95	THR
1	A	103	ASN
1	A	120	THR
1	A	144	HIS
1	A	149	GLN
1	A	150	GLU
1	A	185	GLN

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Mol	Chain	Res	Type
1	A	218	GLN
1	A	259	THR
1	A	292	LEU
1	A	363	VAL
2	B	7	GLU
2	B	11	ARG
2	B	57	LYS
2	B	72	LEU
2	B	76	THR
3	C	42	LYS
3	C	89	GLN
1	D	19	THR
1	D	41	LEU
1	D	45	LEU
1	D	76	SER
1	D	93	LYS
1	D	95	THR
1	D	110	LYS
1	D	120	THR
1	D	144	HIS
1	D	150	GLU
1	D	151	ASN
1	D	157	LYS
1	D	171	GLU
1	D	198	MET
1	D	243	ARG
1	D	245	LEU
1	D	263	ARG
1	D	344	ILE
1	D	355	ILE
1	D	363	VAL
1	D	367	VAL
2	E	7	GLU
2	E	72	LEU
2	E	76	THR
3	F	7	SER
3	F	81	GLU
1	G	13	GLU
1	G	43	ILE
1	G	45	LEU
1	G	70	ILE
1	G	84	GLU

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Mol	Chain	Res	Type
1	G	94	ARG
1	G	95	THR
1	G	99	ARG
1	G	110	LYS
1	G	120	THR
1	G	130	VAL
1	G	144	HIS
1	G	150	GLU
1	G	157	LYS
1	G	159	LEU
1	G	243	ARG
1	G	259	THR
1	G	263	ARG
1	G	265	THR
1	G	273	LEU
1	G	276	LEU
1	G	344	ILE
1	G	363	VAL
2	H	7	GLU
2	H	72	LEU
2	H	76	THR
3	I	70	GLU
3	I	89	GLN
1	J	41	LEU
1	J	45	LEU
1	J	74	CYS
1	J	77	THR
1	J	84	GLU
1	J	95	THR
1	J	120	THR
1	J	148	LYS
1	J	165	SER
1	J	184	VAL
1	J	186	THR
1	J	259	THR
1	J	273	LEU
1	J	295	THR
1	J	304	MET
1	J	325	SER
1	J	363	VAL
1	J	367	VAL
2	K	7	GLU

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Mol	Chain	Res	Type
2	K	57	LYS
2	K	72	LEU
2	K	76	THR
3	L	7	SER
1	M	19	THR
1	M	41	LEU
1	M	45	LEU
1	M	84	GLU
1	M	95	THR
1	M	99	ARG
1	M	103	ASN
1	M	105	CYS
1	M	120	THR
1	M	144	HIS
1	M	150	GLU
1	M	162	ASP
1	M	170	VAL
1	M	243	ARG
1	M	263	ARG
1	M	275	LYS
1	M	320	MET
1	M	361	ASP
1	M	363	VAL
1	M	367	VAL
2	N	7	GLU
2	N	16	SER
2	N	17	GLU
2	N	57	LYS
2	N	72	LEU
2	N	76	THR
2	N	80	SER
3	O	12	SER
3	O	60	SER
3	O	70	GLU
1	P	41	LEU
1	P	45	LEU
1	P	84	GLU
1	P	95	THR
1	P	110	LYS
1	P	120	THR
1	P	150	GLU
1	P	245	LEU

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Mol	Chain	Res	Type
1	P	253	SER
1	P	263	ARG
1	P	320	MET
1	P	326	LYS
1	P	355	ILE
1	P	363	VAL
1	P	392	GLU
2	Q	7	GLU
2	Q	72	LEU
2	Q	76	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	ASN
1	A	192	ASN
1	A	229	HIS
3	C	89	GLN
1	D	144	HIS
1	D	321	GLN
1	G	168	GLN
1	G	218	GLN
1	G	229	HIS
2	H	61	ASN
3	I	89	GLN
1	J	81	HIS
1	J	132	GLN
1	J	218	GLN
1	J	238	HIS
1	J	390	HIS
2	K	59	ASN
1	M	321	GLN
1	M	353	ASN
1	P	103	ASN
1	P	144	HIS
1	P	151	ASN
1	P	229	HIS
2	Q	4	GLN
2	Q	59	ASN
3	R	27	GLN
3	R	92	ASN

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 oligosaccharides 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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	386/395 (97%)	-1.38	0 100 100	32, 46, 76, 95	0
1	D	388/395 (98%)	-1.38	1 (0%) 90 87	32, 50, 87, 103	1 (0%)
1	G	388/395 (98%)	-1.38	0 100 100	31, 48, 80, 111	0
1	J	387/395 (97%)	-1.39	0 100 100	31, 46, 73, 104	1 (0%)
1	M	387/395 (97%)	-1.40	0 100 100	32, 47, 76, 101	0
1	P	387/395 (97%)	-1.39	0 100 100	31, 48, 83, 104	0
2	B	120/120 (100%)	-1.45	0 100 100	30, 46, 70, 90	0
2	E	120/120 (100%)	-1.24	0 100 100	35, 58, 95, 107	0
2	H	120/120 (100%)	-1.22	0 100 100	35, 59, 83, 100	0
2	K	120/120 (100%)	-1.10	0 100 100	32, 64, 97, 106	0
2	N	120/120 (100%)	-1.43	0 100 100	32, 45, 68, 78	1 (0%)
2	Q	120/120 (100%)	-1.24	0 100 100	35, 60, 85, 94	0
3	C	107/107 (100%)	-1.44	0 100 100	35, 52, 77, 89	0
3	F	107/107 (100%)	-1.28	0 100 100	40, 57, 84, 98	0
3	I	107/107 (100%)	-1.43	0 100 100	38, 53, 71, 76	0
3	L	106/107 (99%)	-1.41	0 100 100	39, 59, 82, 113	0
3	O	107/107 (100%)	-1.42	0 100 100	33, 46, 69, 82	0
3	R	107/107 (100%)	-1.37	0 100 100	35, 50, 76, 91	0
All	All	3684/3732 (98%)	-1.37	1 (0%) 100 100	30, 49, 83, 113	3 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	76	SER	2.1

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 oligosaccharides 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.