Full wwPDB X-ray Structure Validation Report ⓘ

Jan 28, 2024 – 01:01 AM EST

PDB ID	:	1DM5
Title	:	ANNEXIN XII E105K HOMOHEXAMER CRYSTAL STRUCTURE
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Deposited on	:	1999-12-13
Resolution	:	1.93 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:

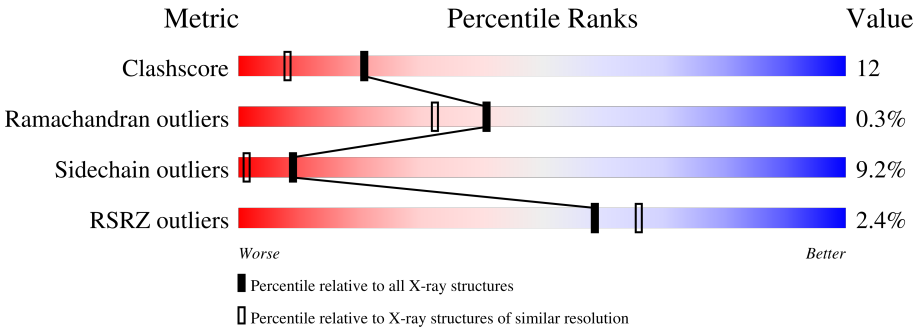
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 1.93 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))
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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	315	2% 70% 26% ·
1	B	315	3% 73% 23% · ·
1	C	315	2% 74% 22% ·
1	D	315	3% 73% 23% ·
1	E	315	2% 64% 32% ·
1	F	315	2% 68% 27% 5%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CA	E	1125	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 15709 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 ANNEXIN XII E105K MUTANT HOMOHEXAMER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	0	0	0
			2462	1544	429	482	7			
1	B	315	Total	C	N	O	S	0	0	0
			2462	1544	429	482	7			
1	C	315	Total	C	N	O	S	0	0	0
			2462	1544	429	482	7			
1	D	315	Total	C	N	O	S	0	0	0
			2462	1544	429	482	7			
1	E	315	Total	C	N	O	S	0	0	0
			2462	1544	429	482	7			
1	F	315	Total	C	N	O	S	0	0	0
			2462	1544	429	482	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	105	LYS	GLU	engineered mutation	UNP P26256
B	105	LYS	GLU	engineered mutation	UNP P26256
C	105	LYS	GLU	engineered mutation	UNP P26256
D	105	LYS	GLU	engineered mutation	UNP P26256
E	105	LYS	GLU	engineered mutation	UNP P26256
F	105	LYS	GLU	engineered mutation	UNP P26256

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		
2	B	2	Total	Ca	0	0
			2	2		
2	C	2	Total	Ca	0	0
			2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	2	Total Ca 2 2	0	0
2	E	2	Total Ca 2 2	0	0
2	F	1	Total Ca 1 1	0	0

- Molecule 3 is water.

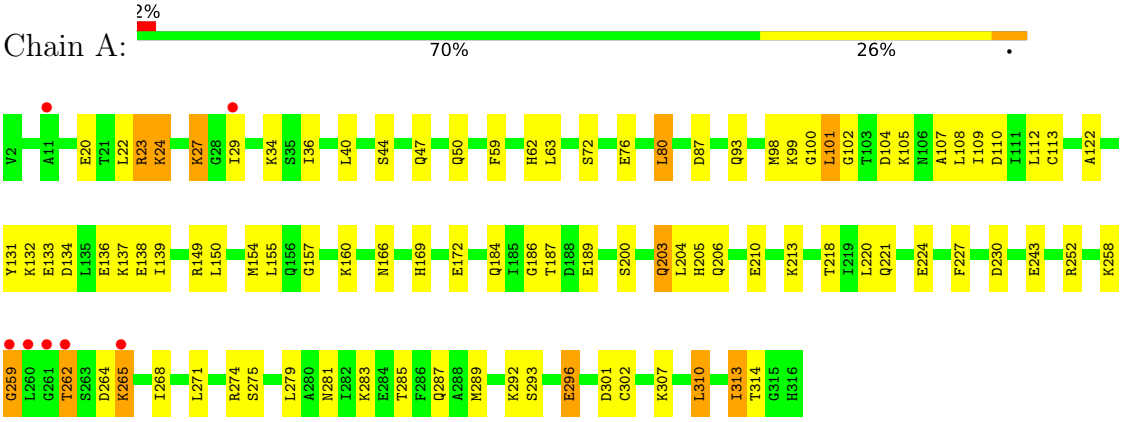
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	140	Total O 140 140	0	0
3	B	193	Total O 193 193	0	0
3	C	173	Total O 173 173	0	0
3	D	152	Total O 152 152	0	0
3	E	117	Total O 117 117	0	0
3	F	151	Total O 151 151	0	0

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.

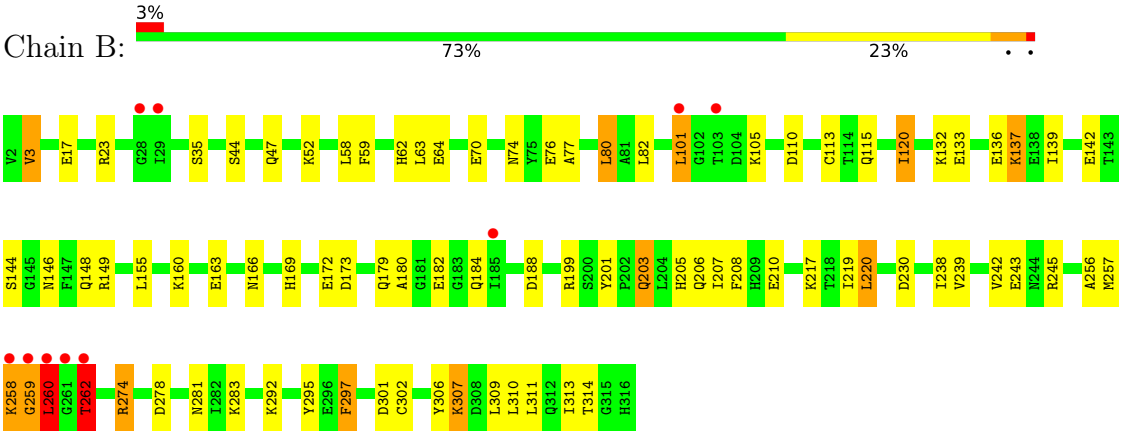
• Molecule 1: ANNEXIN XII E105K MUTANT HOMOHEXAMER

Chain A:



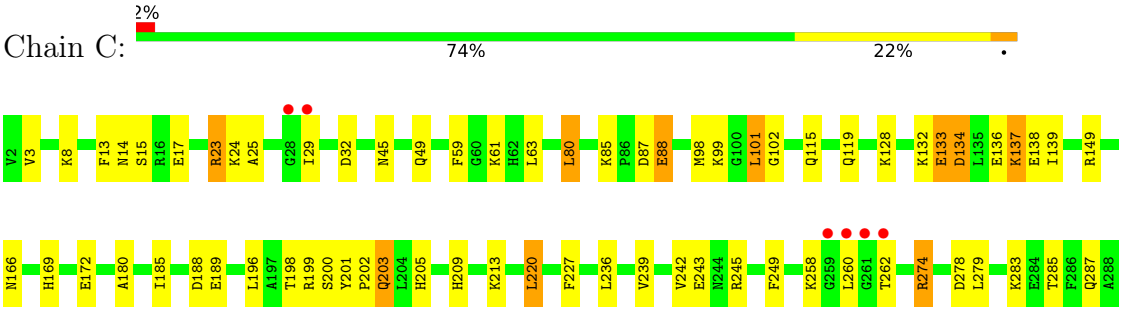
• Molecule 1: ANNEXIN XII E105K MUTANT HOMOHEXAMER

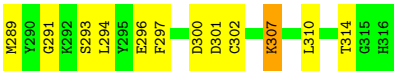
Chain B:



• Molecule 1: ANNEXIN XII E105K MUTANT HOMOHEXAMER

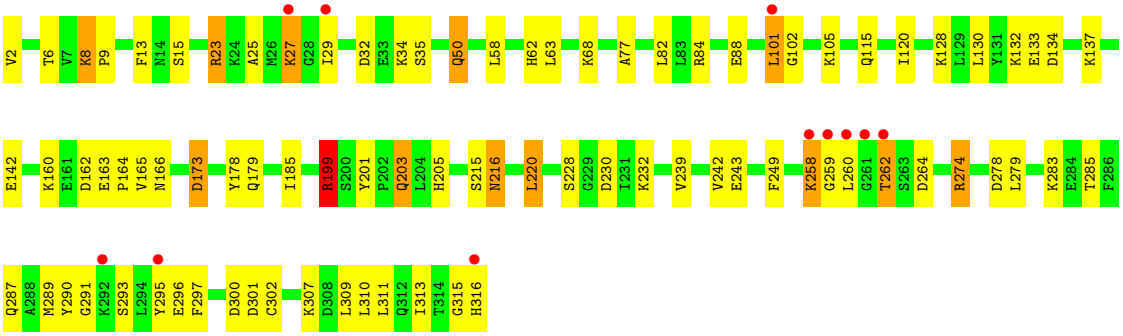
Chain C:





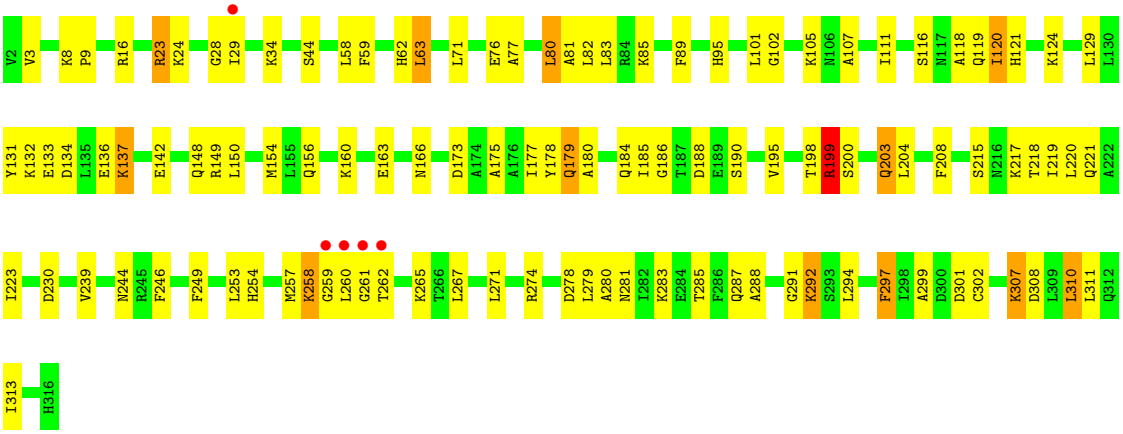
• Molecule 1: ANNEXIN XII E105K MUTANT HOMOHEXAMER

Chain D:



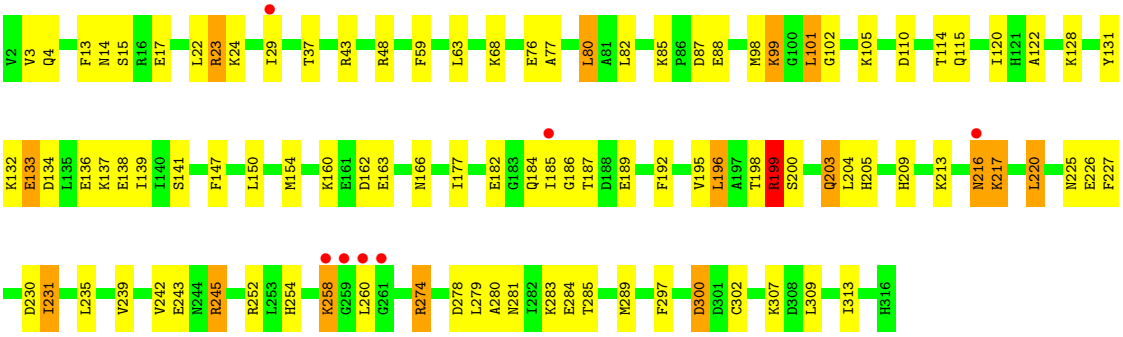
• Molecule 1: ANNEXIN XII E105K MUTANT HOMOHEXAMER

Chain E:



• Molecule 1: ANNEXIN XII E105K MUTANT HOMOHEXAMER

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	68.94Å 162.54Å 188.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.93 81.63 – 1.90	Depositor EDS
% Data completeness (in resolution range)	92.5 (10.00-1.93) 90.3 (81.63-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.50 (at 1.90Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.208 , 0.263 0.211 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	21.3	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 70.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	15709	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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 (i)

5.1 Standard geometry (i)

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

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	0.32	0/2498	0.79	0/3360
1	B	0.32	0/2498	0.85	1/3360 (0.0%)
1	C	0.32	0/2498	0.87	6/3360 (0.2%)
1	D	0.32	0/2498	0.88	4/3360 (0.1%)
1	E	0.30	0/2498	0.88	9/3360 (0.3%)
1	F	0.32	0/2498	0.84	5/3360 (0.1%)
All	All	0.32	0/14988	0.85	25/20160 (0.1%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	199	ARG	NE-CZ-NH1	13.24	126.92	120.30
1	E	199	ARG	CD-NE-CZ	12.15	140.61	123.60
1	E	199	ARG	NE-CZ-NH2	-9.77	115.42	120.30
1	D	199	ARG	CD-NE-CZ	9.71	137.19	123.60
1	F	199	ARG	NE-CZ-NH1	9.68	125.14	120.30
1	E	149	ARG	NE-CZ-NH2	9.22	124.91	120.30
1	C	199	ARG	NE-CZ-NH2	9.10	124.85	120.30
1	B	260	LEU	C-N-CA	9.03	141.26	122.30
1	F	199	ARG	NE-CZ-NH2	-8.52	116.04	120.30
1	E	308	ASP	CB-CG-OD1	8.46	125.92	118.30
1	E	199	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	D	199	ARG	NE-CZ-NH2	-8.21	116.19	120.30
1	C	149	ARG	CD-NE-CZ	7.32	133.85	123.60
1	F	48	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	F	199	ARG	CD-NE-CZ	7.09	133.52	123.60
1	E	149	ARG	NE-CZ-NH1	-6.82	116.89	120.30
1	C	149	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	E	16	ARG	NE-CZ-NH1	-6.54	117.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	199	ARG	NE-CZ-NH1	-6.47	117.06	120.30
1	E	149	ARG	CD-NE-CZ	6.25	132.35	123.60
1	C	199	ARG	CD-NE-CZ	5.40	131.16	123.60
1	C	149	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	D	173	ASP	CB-CG-OD2	5.33	123.10	118.30
1	E	308	ASP	CB-CG-OD2	-5.07	113.73	118.30
1	F	43	ARG	NE-CZ-NH2	5.00	122.80	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2462	0	2457	71	0
1	B	2462	0	2457	64	0
1	C	2462	0	2457	50	0
1	D	2462	0	2457	69	0
1	E	2462	0	2457	75	0
1	F	2462	0	2457	65	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	1	0	0	0	0
3	A	140	0	0	7	0
3	B	193	0	0	5	0
3	C	173	0	0	6	0
3	D	152	0	0	3	0
3	E	117	0	0	9	0
3	F	151	0	0	6	0
All	All	15709	0	14742	364	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 12.

All (364) 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:260:LEU:CD1	1:D:260:LEU:HD13	1.45	1.44
1:B:260:LEU:HD12	1:D:260:LEU:CD1	1.59	1.30
1:B:260:LEU:CD1	1:D:260:LEU:CD1	2.19	1.10
1:F:82:LEU:HD11	1:F:313:ILE:HD11	1.39	1.01
1:E:82:LEU:HD11	1:E:313:ILE:HD11	1.44	1.00
1:B:82:LEU:HD11	1:B:313:ILE:HD11	1.46	0.94
1:D:166:ASN:H	1:D:203:GLN:HE22	1.20	0.90
1:C:85:LYS:HB2	1:C:88:GLU:HG3	1.53	0.89
1:B:260:LEU:HD13	1:D:260:LEU:HD13	1.57	0.87
1:E:132:LYS:HE2	3:E:1163:HOH:O	1.76	0.85
1:B:260:LEU:HD13	1:D:260:LEU:CD1	2.06	0.85
1:B:260:LEU:HD12	1:D:260:LEU:HD13	0.84	0.84
1:E:3:VAL:HA	1:E:281:ASN:HD21	1.41	0.83
1:D:82:LEU:HD11	1:D:313:ILE:HD11	1.60	0.82
1:E:166:ASN:H	1:E:203:GLN:HE22	1.26	0.80
1:A:224:GLU:HG2	3:A:1261:HOH:O	1.84	0.77
1:B:166:ASN:H	1:B:203:GLN:HE22	1.31	0.76
1:D:279:LEU:O	1:D:283:LYS:HG3	1.86	0.76
1:A:169:HIS:HA	1:A:172:GLU:OE2	1.85	0.76
1:E:279:LEU:O	1:E:283:LYS:HG3	1.85	0.76
1:A:265:LYS:HE2	1:A:268:ILE:HD12	1.67	0.75
1:D:285:THR:O	1:D:289:MET:HG3	1.87	0.75
1:C:25:ALA:HB1	1:C:32:ASP:HB3	1.69	0.75
1:D:293:SER:OG	1:D:296:GLU:HG3	1.88	0.74
1:C:166:ASN:H	1:C:203:GLN:HE22	1.36	0.74
1:B:203:GLN:HE21	1:B:203:GLN:HA	1.51	0.74
1:A:166:ASN:H	1:A:203:GLN:HE22	1.36	0.73
1:E:3:VAL:HA	1:E:281:ASN:ND2	2.02	0.73
1:C:279:LEU:O	1:C:283:LYS:HG3	1.88	0.73
1:E:179:GLN:HA	1:E:179:GLN:HE21	1.55	0.72
1:F:274:ARG:HD3	1:F:278:ASP:OD1	1.90	0.72
1:D:307:LYS:O	1:D:311:LEU:HG	1.90	0.72
1:A:101:LEU:HD13	1:E:77:ALA:HB1	1.72	0.71
1:E:254:HIS:NE2	1:E:258:LYS:HD3	2.05	0.71
1:A:271:LEU:HD12	1:A:310:LEU:HG	1.72	0.71
1:E:257:MET:HA	1:E:262:THR:HG23	1.72	0.71
1:A:285:THR:O	1:A:289:MET:HG3	1.91	0.70
1:B:302:CYS:HB2	1:B:307:LYS:HB2	1.73	0.70
1:C:87:ASP:HB2	3:C:1292:HOH:O	1.92	0.70
1:B:219:ILE:HG23	1:B:220:LEU:HD13	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:GLN:HE21	1:C:203:GLN:HA	1.58	0.69
1:E:132:LYS:HG2	3:E:1163:HOH:O	1.91	0.69
1:A:206:GLN:O	1:A:210:GLU:HG2	1.94	0.68
1:D:115:GLN:HB2	1:D:120:ILE:HG12	1.75	0.68
1:F:189:GLU:OE2	1:F:231:ILE:HD11	1.93	0.67
1:A:292:LYS:HG2	1:A:296:GLU:OE1	1.94	0.67
1:B:256:ALA:O	1:B:262:THR:HA	1.94	0.67
1:D:84:ARG:NH1	1:D:88:GLU:OE2	2.28	0.67
1:B:105:LYS:HD2	1:B:230:ASP:OD1	1.95	0.67
1:D:258:LYS:NZ	1:D:259:GLY:H	1.93	0.66
1:A:203:GLN:HA	1:A:203:GLN:HE21	1.60	0.66
1:E:184:GLN:HG3	1:E:186:GLY:O	1.95	0.66
1:B:274:ARG:HD3	1:B:278:ASP:OD1	1.95	0.66
1:E:274:ARG:HD3	1:E:278:ASP:OD1	1.94	0.66
1:D:13:PHE:HA	3:D:1237:HOH:O	1.96	0.66
1:F:163:GLU:HB3	1:F:200:SER:HB3	1.78	0.66
1:E:166:ASN:H	1:E:203:GLN:NE2	1.92	0.65
1:A:283:LYS:HD3	1:A:314:THR:HG22	1.79	0.65
1:E:63:LEU:HD13	1:E:83:LEU:HD11	1.78	0.65
1:E:203:GLN:HE21	1:E:203:GLN:HA	1.62	0.65
1:A:258:LYS:NZ	1:A:258:LYS:HA	2.13	0.64
1:B:292:LYS:HD3	1:B:297:PHE:CD2	2.33	0.64
1:B:208:PHE:CE1	1:B:239:VAL:HG13	2.33	0.64
1:F:279:LEU:O	1:F:283:LYS:HG3	1.98	0.64
1:A:149:ARG:HD3	1:C:61:LYS:HE3	1.80	0.63
1:E:120:ILE:HD12	1:E:154:MET:O	1.98	0.63
1:E:199:ARG:HB2	1:E:204:LEU:HG	1.79	0.63
1:D:203:GLN:HE21	1:D:203:GLN:HA	1.64	0.63
1:E:175:ALA:O	1:E:179:GLN:HG2	1.99	0.63
1:F:99:LYS:HD3	1:F:99:LYS:N	2.14	0.63
1:B:144:SER:HA	1:B:148:GLN:HE21	1.64	0.63
1:C:220:LEU:HD12	1:C:236:LEU:HD22	1.81	0.62
1:D:274:ARG:HD3	1:D:278:ASP:OD1	1.99	0.62
1:E:173:ASP:OD1	1:E:199:ARG:HD2	1.98	0.62
1:F:203:GLN:HE21	1:F:203:GLN:HA	1.63	0.62
1:D:166:ASN:H	1:D:203:GLN:NE2	1.95	0.62
1:F:76:GLU:HG2	1:F:80:LEU:HD22	1.80	0.62
1:B:17:GLU:OE2	3:B:1241:HOH:O	2.16	0.62
1:D:173:ASP:OD1	1:D:199:ARG:HD3	1.99	0.62
1:C:302:CYS:HB2	1:C:307:LYS:HB2	1.81	0.62
1:B:101:LEU:HD13	1:D:77:ALA:HB1	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:ASN:HD22	1:D:216:ASN:H	1.46	0.61
1:A:98:MET:HB3	1:A:99:LYS:HE2	1.82	0.61
1:D:220:LEU:HD13	1:D:239:VAL:HG11	1.82	0.61
1:C:115:GLN:OE1	1:C:119:GLN:HB3	2.00	0.61
1:A:36:ILE:O	1:A:40:LEU:HG	2.00	0.61
1:A:80:LEU:HD23	1:E:102:GLY:HA2	1.83	0.61
1:E:208:PHE:CE1	1:E:239:VAL:HG13	2.36	0.60
1:A:293:SER:OG	1:A:296:GLU:HG3	2.01	0.60
1:D:258:LYS:HZ1	1:D:259:GLY:H	1.49	0.60
1:A:166:ASN:H	1:A:203:GLN:NE2	2.00	0.60
1:C:166:ASN:H	1:C:203:GLN:NE2	2.00	0.59
3:C:1255:HOH:O	1:F:68:LYS:HE2	2.02	0.59
1:D:105:LYS:HD2	1:D:230:ASP:OD1	2.02	0.59
1:E:107:ALA:O	1:E:111:ILE:HG13	2.02	0.59
1:E:271:LEU:HD12	1:E:310:LEU:HG	1.85	0.59
1:A:189:GLU:HG3	1:A:227:PHE:HE1	1.67	0.59
1:E:292:LYS:HD3	1:E:297:PHE:CE2	2.37	0.59
1:A:136:GLU:HA	1:A:155:LEU:HD13	1.85	0.59
1:B:260:LEU:HD12	1:D:260:LEU:HD11	1.75	0.59
1:F:216:ASN:H	1:F:216:ASN:ND2	2.01	0.58
1:A:264:ASP:O	1:A:268:ILE:HG13	2.02	0.58
1:B:144:SER:HA	1:B:148:GLN:NE2	2.18	0.58
1:E:280:ALA:O	1:E:283:LYS:HB2	2.03	0.58
1:A:62:HIS:HE1	1:B:136:GLU:OE2	1.87	0.58
1:C:220:LEU:HD12	1:C:236:LEU:CD2	2.34	0.57
1:E:271:LEU:CD1	1:E:310:LEU:HG	2.33	0.57
1:F:105:LYS:HD2	1:F:230:ASP:OD1	2.02	0.57
1:B:62:HIS:HE1	1:C:136:GLU:OE2	1.88	0.57
1:A:23:ARG:HG3	1:A:59:PHE:CZ	2.40	0.57
1:E:254:HIS:CD2	1:E:258:LYS:HD3	2.38	0.57
1:E:62:HIS:HE1	1:F:136:GLU:OE2	1.86	0.57
1:F:150:LEU:O	1:F:154:MET:HG2	2.04	0.57
1:D:62:HIS:HE1	1:E:136:GLU:OE2	1.87	0.57
1:F:182:GLU:OE2	1:F:217:LYS:HD2	2.03	0.57
1:B:283:LYS:HD3	1:B:314:THR:HG22	1.86	0.56
1:E:23:ARG:HG3	1:E:59:PHE:CE2	2.41	0.56
1:A:44:SER:OG	1:A:47:GLN:HG3	2.06	0.56
1:C:25:ALA:CB	1:C:32:ASP:HB3	2.35	0.56
1:D:262:THR:HB	1:D:264:ASP:OD1	2.06	0.56
1:B:205:HIS:HD2	1:B:243:GLU:OE2	1.89	0.56
1:A:101:LEU:HD11	1:E:81:ALA:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:LYS:O	1:A:200:SER:HB3	2.06	0.55
1:B:77:ALA:HB1	1:D:101:LEU:HD13	1.89	0.55
1:A:102:GLY:HA2	1:E:80:LEU:HD23	1.89	0.55
1:E:23:ARG:HG3	1:E:59:PHE:CZ	2.42	0.55
1:D:13:PHE:CZ	1:D:15:SER:HB3	2.42	0.55
1:A:205:HIS:HD2	1:A:243:GLU:OE2	1.89	0.55
1:D:88:GLU:HG2	1:D:130:LEU:HD11	1.88	0.55
1:F:3:VAL:HA	1:F:281:ASN:HD21	1.71	0.55
1:C:285:THR:O	1:C:289:MET:HG3	2.07	0.54
1:E:116:SER:OG	1:E:119:GLN:HB2	2.08	0.54
1:D:205:HIS:HD2	1:D:243:GLU:OE2	1.90	0.54
1:D:295:TYR:CD1	1:D:316:HIS:HA	2.43	0.54
1:C:101:LEU:HD13	1:F:77:ALA:HB1	1.90	0.54
1:C:283:LYS:HD3	1:C:314:THR:CG2	2.37	0.54
1:E:62:HIS:HD2	3:E:1208:HOH:O	1.90	0.54
1:D:285:THR:HG22	1:D:289:MET:SD	2.48	0.54
1:F:205:HIS:HD2	1:F:243:GLU:OE2	1.91	0.54
1:C:205:HIS:HD2	1:C:243:GLU:OE2	1.90	0.54
1:C:220:LEU:HD13	1:C:239:VAL:HG11	1.89	0.54
1:A:283:LYS:HD3	1:A:314:THR:CG2	2.37	0.53
1:C:23:ARG:HG3	1:C:59:PHE:CZ	2.43	0.53
1:A:279:LEU:O	1:A:283:LYS:HG3	2.09	0.53
1:F:300:ASP:HB3	3:F:1275:HOH:O	2.09	0.53
1:E:299:ALA:O	1:E:307:LYS:HE3	2.08	0.53
1:C:262:THR:HG23	1:C:301:ASP:OD2	2.09	0.53
1:F:87:ASP:HB2	3:F:1258:HOH:O	2.08	0.53
1:B:262:THR:OG1	1:B:301:ASP:OD2	2.24	0.52
1:C:137:LYS:HE2	3:C:1259:HOH:O	2.08	0.52
1:B:23:ARG:HG2	1:B:59:PHE:CZ	2.44	0.52
1:C:202:PRO:HG2	3:C:1157:HOH:O	2.09	0.52
1:C:128:LYS:NZ	1:C:134:ASP:OD2	2.33	0.52
1:C:274:ARG:HD3	1:C:278:ASP:OD1	2.09	0.52
1:E:150:LEU:O	1:E:154:MET:HG2	2.09	0.52
1:A:87:ASP:OD2	1:A:122:ALA:HB1	2.10	0.52
1:D:6:THR:CG2	1:D:283:LYS:HE2	2.40	0.52
1:D:2:VAL:O	1:D:2:VAL:HG13	2.09	0.52
1:B:180:ALA:HB1	1:B:188:ASP:HB3	1.92	0.52
1:A:258:LYS:HG3	1:A:259:GLY:H	1.75	0.51
1:C:283:LYS:HD3	1:C:314:THR:HG22	1.91	0.51
1:F:302:CYS:HB2	1:F:307:LYS:HB2	1.91	0.51
1:F:220:LEU:HD13	1:F:239:VAL:HG11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:GLU:OE2	1:C:138:GLU:HG2	2.10	0.51
1:A:184:GLN:HG3	1:A:186:GLY:O	2.10	0.51
1:A:265:LYS:HE2	1:A:268:ILE:CD1	2.37	0.51
1:B:70:GLU:HG2	3:B:1290:HOH:O	2.11	0.51
1:B:257:MET:O	1:B:258:LYS:O	2.28	0.51
1:B:260:LEU:HB3	1:D:260:LEU:HB3	1.93	0.50
1:B:309:LEU:O	1:B:313:ILE:HD12	2.10	0.50
1:E:249:PHE:CE2	1:E:274:ARG:HD2	2.46	0.50
1:B:62:HIS:HD2	3:B:1252:HOH:O	1.94	0.50
1:F:285:THR:O	1:F:289:MET:HG3	2.11	0.50
1:A:102:GLY:CA	1:E:80:LEU:HD23	2.42	0.50
1:E:124:LYS:HE3	3:E:1242:HOH:O	2.11	0.50
1:F:23:ARG:HG3	1:F:59:PHE:CE2	2.47	0.50
1:F:14:ASN:CG	1:F:17:GLU:HG3	2.32	0.50
1:F:133:GLU:OE2	1:F:138:GLU:OE2	2.30	0.50
1:D:8:LYS:HG2	1:D:9:PRO:HD2	1.93	0.50
1:F:98:MET:SD	1:F:139:ILE:HD13	2.52	0.50
1:B:302:CYS:CB	1:B:307:LYS:HB2	2.42	0.50
1:F:231:ILE:HD13	1:F:235:LEU:HG	1.94	0.50
1:E:23:ARG:HH11	1:E:23:ARG:HG2	1.77	0.49
1:C:13:PHE:CZ	1:C:15:SER:HB3	2.48	0.49
1:D:309:LEU:O	1:D:313:ILE:HD12	2.12	0.49
1:B:182:GLU:CD	1:B:217:LYS:HD2	2.33	0.49
1:E:262:THR:OG1	1:E:301:ASP:OD2	2.30	0.49
1:F:85:LYS:HE3	1:F:88:GLU:OE1	2.13	0.49
1:F:131:TYR:O	1:F:132:LYS:HB2	2.12	0.49
1:B:166:ASN:H	1:B:203:GLN:NE2	2.05	0.49
1:F:3:VAL:HG23	3:F:1273:HOH:O	2.11	0.49
1:D:249:PHE:CE2	1:D:274:ARG:HD2	2.48	0.49
1:F:254:HIS:NE2	1:F:258:LYS:HD3	2.28	0.49
1:A:134:ASP:HB3	1:A:137:LYS:HG2	1.94	0.49
1:B:179:GLN:O	1:B:184:GLN:HG2	2.13	0.49
1:F:187:THR:OG1	1:F:226:GLU:OE2	2.30	0.48
1:B:160:LYS:HD3	1:B:163:GLU:HB2	1.94	0.48
1:B:201:TYR:CG	1:B:242:VAL:HG22	2.47	0.48
1:A:98:MET:SD	1:A:139:ILE:HD13	2.53	0.48
1:A:27:LYS:HE2	3:A:1218:HOH:O	2.13	0.48
1:A:100:GLY:N	3:A:1239:HOH:O	2.45	0.48
1:D:8:LYS:HE2	1:D:9:PRO:HD2	1.94	0.48
1:D:164:PRO:HD2	3:D:1159:HOH:O	2.12	0.48
1:F:3:VAL:HA	1:F:281:ASN:ND2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:289:MET:HE2	1:D:290:TYR:CE2	2.48	0.48
1:A:184:GLN:HB3	3:A:1159:HOH:O	2.13	0.48
1:B:44:SER:OG	1:B:47:GLN:HG3	2.13	0.48
1:C:8:LYS:HE2	3:C:1278:HOH:O	2.13	0.48
1:E:244:ASN:OD1	1:E:246:PHE:HB2	2.13	0.48
1:F:115:GLN:HB2	1:F:120:ILE:HG12	1.94	0.48
1:C:293:SER:OG	1:C:296:GLU:HG3	2.13	0.48
1:B:139:ILE:HG13	1:B:155:LEU:HD11	1.96	0.48
1:D:160:LYS:HG2	1:D:163:GLU:HB2	1.96	0.48
1:E:121:HIS:HE1	1:E:156:GLN:O	1.97	0.47
1:F:87:ASP:OD2	1:F:122:ALA:HB1	2.14	0.47
1:E:58:LEU:HG	1:F:198:THR:HG21	1.96	0.47
1:A:110:ASP:CG	1:A:252:ARG:HE	2.17	0.47
1:F:209:HIS:NE2	1:F:213:LYS:HE2	2.30	0.47
1:C:189:GLU:HG2	1:C:227:PHE:CE1	2.50	0.47
1:E:102:GLY:O	3:E:1197:HOH:O	2.20	0.47
1:F:192:PHE:O	1:F:196:LEU:HB2	2.14	0.47
1:B:80:LEU:HD23	1:D:102:GLY:HA2	1.96	0.47
1:B:206:GLN:O	1:B:210:GLU:HG2	2.14	0.47
1:B:258:LYS:HA	1:B:258:LYS:NZ	2.30	0.47
1:C:14:ASN:CG	1:C:17:GLU:HG3	2.34	0.47
1:D:178:TYR:CE1	1:D:215:SER:HB2	2.49	0.47
1:E:177:ILE:HD11	1:E:195:VAL:HG11	1.96	0.47
1:D:58:LEU:HD23	1:E:198:THR:HG21	1.97	0.47
1:D:295:TYR:HD1	1:D:315:GLY:O	1.97	0.47
1:E:142:GLU:OE2	1:E:142:GLU:HA	2.15	0.47
1:A:149:ARG:HE	1:C:61:LYS:HE2	1.80	0.46
1:B:295:TYR:CE1	1:B:311:LEU:HD22	2.49	0.46
1:B:307:LYS:NZ	3:B:1271:HOH:O	2.47	0.46
1:F:177:ILE:HD11	1:F:195:VAL:HG11	1.97	0.46
1:A:218:THR:HG23	1:A:221:GLN:OE1	2.15	0.46
1:C:180:ALA:HB1	1:C:188:ASP:HB3	1.97	0.46
1:B:258:LYS:O	1:B:259:GLY:O	2.33	0.46
1:F:105:LYS:HD2	1:F:230:ASP:CG	2.36	0.46
1:B:105:LYS:HD2	1:B:230:ASP:CG	2.35	0.46
1:C:99:LYS:HE3	1:C:138:GLU:OE1	2.15	0.46
1:E:219:ILE:HG13	1:E:223:ILE:HD12	1.98	0.46
1:A:150:LEU:O	1:A:154:MET:HG2	2.16	0.46
1:C:98:MET:SD	1:C:139:ILE:HD13	2.55	0.46
1:A:262:THR:O	1:A:264:ASP:N	2.49	0.46
1:F:4:GLN:O	1:F:280:ALA:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:ASN:OD1	1:B:149:ARG:NH1	2.49	0.46
1:A:109:ILE:O	1:A:113:CYS:HB2	2.16	0.46
1:D:15:SER:OG	1:D:50:GLN:NE2	2.49	0.46
1:E:285:THR:O	1:E:288:ALA:HB3	2.17	0.45
1:F:199:ARG:HB2	1:F:204:LEU:HG	1.98	0.45
1:D:201:TYR:CG	1:D:242:VAL:HG22	2.52	0.45
1:A:271:LEU:HB3	1:A:313:ILE:HD11	1.98	0.45
1:D:6:THR:HG22	1:D:283:LYS:HE2	1.99	0.45
1:F:216:ASN:OD1	1:F:217:LYS:HG3	2.16	0.45
1:F:196:LEU:HD23	1:F:235:LEU:HD22	1.98	0.45
1:B:206:GLN:NE2	1:B:210:GLU:OE2	2.50	0.45
1:E:259:GLY:C	1:E:261:GLY:H	2.20	0.45
1:B:137:LYS:NZ	1:E:137:LYS:NZ	2.65	0.45
1:E:217:LYS:HB3	1:E:221:GLN:HB2	1.99	0.45
1:A:258:LYS:O	1:A:259:GLY:O	2.35	0.45
1:A:293:SER:H	1:A:296:GLU:CD	2.20	0.45
1:E:71:LEU:HB2	1:E:76:GLU:HG3	1.99	0.45
1:A:20:GLU:OE1	1:A:24:LYS:NZ	2.50	0.44
1:D:178:TYR:HE1	1:D:215:SER:HB2	1.82	0.44
1:F:281:ASN:OD1	1:F:281:ASN:N	2.50	0.44
1:D:295:TYR:CZ	1:D:316:HIS:NE2	2.86	0.44
1:B:169:HIS:HA	1:B:172:GLU:OE1	2.17	0.44
1:C:3:VAL:HG22	3:C:1276:HOH:O	2.16	0.44
1:D:287:GLN:NE2	1:D:291:GLY:O	2.50	0.44
1:F:189:GLU:HG2	1:F:227:PHE:CE1	2.53	0.44
1:B:142:GLU:OE2	1:D:68:LYS:HE2	2.17	0.44
1:D:105:LYS:HD2	1:D:230:ASP:CG	2.38	0.44
1:A:93:GLN:NE2	3:A:1210:HOH:O	2.51	0.44
1:C:200:SER:HB2	1:C:202:PRO:HD2	1.99	0.44
1:F:110:ASP:OD2	1:F:252:ARG:NE	2.51	0.44
1:A:187:THR:HG22	1:A:189:GLU:N	2.33	0.44
1:E:180:ALA:HB1	1:E:188:ASP:HB3	2.00	0.44
1:F:220:LEU:HD12	1:F:220:LEU:HA	1.76	0.44
1:F:230:ASP:HB2	3:F:1267:HOH:O	2.16	0.44
1:E:9:PRO:HA	1:E:44:SER:HB3	1.99	0.44
1:E:63:LEU:HD13	1:E:83:LEU:CD1	2.48	0.44
1:A:62:HIS:HD2	3:A:1234:HOH:O	2.00	0.43
1:B:292:LYS:HD3	1:B:297:PHE:CE2	2.53	0.43
1:D:165:VAL:HA	1:D:203:GLN:NE2	2.33	0.43
1:D:228:SER:HA	1:D:232:LYS:HD3	2.00	0.43
1:D:258:LYS:HD2	1:D:258:LYS:HA	1.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:262:THR:HG23	1:D:301:ASP:OD2	2.17	0.43
1:E:307:LYS:HG2	1:E:311:LEU:CD1	2.48	0.43
1:A:271:LEU:CD1	1:A:310:LEU:HG	2.43	0.43
1:B:76:GLU:HG2	1:B:80:LEU:HD22	2.00	0.43
1:B:173:ASP:OD1	1:B:207:ILE:HD11	2.18	0.43
1:D:23:ARG:O	1:D:27:LYS:HB2	2.18	0.43
1:E:218:THR:HG21	3:E:1222:HOH:O	2.18	0.43
1:A:258:LYS:HA	1:A:258:LYS:CE	2.48	0.43
1:D:302:CYS:C	1:D:307:LYS:HB2	2.39	0.43
1:C:283:LYS:HG2	1:C:294:LEU:HD23	1.99	0.43
1:C:45:ASN:O	1:C:49:GLN:HG2	2.18	0.43
1:B:3:VAL:HA	1:B:281:ASN:HD21	1.83	0.43
1:D:25:ALA:HB1	1:D:32:ASP:HB3	2.00	0.43
1:C:169:HIS:HA	1:C:172:GLU:OE2	2.19	0.43
1:C:262:THR:CG2	1:C:301:ASP:OD2	2.66	0.43
1:F:22:LEU:HD23	1:F:22:LEU:HA	1.85	0.43
1:E:195:VAL:O	1:E:199:ARG:HG2	2.19	0.43
1:F:114:THR:O	1:F:245:ARG:NH1	2.52	0.43
1:F:166:ASN:H	1:F:203:GLN:HE22	1.66	0.43
1:A:157:GLY:N	3:A:1212:HOH:O	2.52	0.43
1:E:28:GLY:O	3:E:1234:HOH:O	2.20	0.43
1:E:118:ALA:HB2	3:E:1171:HOH:O	2.18	0.43
1:E:287:GLN:NE2	1:E:291:GLY:O	2.50	0.43
1:C:287:GLN:NE2	1:C:291:GLY:O	2.52	0.42
1:A:131:TYR:O	1:A:132:LYS:HB3	2.18	0.42
1:C:80:LEU:HD23	1:F:102:GLY:HA2	2.01	0.42
1:A:76:GLU:HG2	1:A:80:LEU:HD22	2.01	0.42
1:E:105:LYS:HD2	1:E:230:ASP:CG	2.40	0.42
1:F:98:MET:C	1:F:99:LYS:HD3	2.40	0.42
1:E:148:GLN:NE2	3:E:1217:HOH:O	2.52	0.42
1:C:102:GLY:HA2	1:F:80:LEU:HD23	2.01	0.42
1:F:13:PHE:CZ	1:F:15:SER:HB3	2.54	0.42
1:B:110:ASP:CB	3:B:1299:HOH:O	2.67	0.42
1:F:141:SER:HB3	3:F:1237:HOH:O	2.20	0.42
1:F:189:GLU:HG2	1:F:227:PHE:HE1	1.83	0.42
1:F:147:PHE:CD1	1:F:230:ASP:HB3	2.55	0.41
1:A:99:LYS:HE3	1:A:138:GLU:OE1	2.20	0.41
1:C:200:SER:CB	1:C:202:PRO:HD2	2.51	0.41
1:D:179:GLN:NE2	3:D:1250:HOH:O	2.52	0.41
1:F:160:LYS:NZ	1:F:162:ASP:OD1	2.52	0.41
1:F:184:GLN:HG3	1:F:186:GLY:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:LEU:O	1:A:112:LEU:HB2	2.20	0.41
1:A:136:GLU:HA	1:A:155:LEU:CD1	2.48	0.41
1:D:293:SER:HG	1:D:296:GLU:HG3	1.81	0.41
1:E:267:LEU:O	1:E:271:LEU:HG	2.21	0.41
1:F:37:THR:HG23	1:F:309:LEU:HD13	2.02	0.41
1:D:274:ARG:NH1	1:D:278:ASP:OD2	2.52	0.41
1:E:160:LYS:O	1:E:200:SER:HB3	2.20	0.41
1:A:293:SER:N	1:A:296:GLU:OE1	2.51	0.41
1:D:220:LEU:HD12	1:D:220:LEU:HA	1.89	0.41
1:A:187:THR:HG22	1:A:189:GLU:OE2	2.20	0.41
1:C:209:HIS:CD2	1:C:213:LYS:HE3	2.56	0.41
1:A:271:LEU:O	1:A:275:SER:HB3	2.20	0.41
1:B:74:ASN:HB3	1:B:306:TYR:CE1	2.55	0.41
1:E:178:TYR:CE1	1:E:215:SER:HB2	2.55	0.41
1:F:242:VAL:HG12	1:F:243:GLU:OE2	2.20	0.41
1:A:104:ASP:O	1:A:107:ALA:HB3	2.21	0.41
1:A:105:LYS:HD2	1:A:230:ASP:OD1	2.21	0.41
1:A:302:CYS:O	1:A:307:LYS:HD2	2.21	0.41
1:B:52:LYS:HE3	1:B:64:GLU:OE2	2.20	0.41
1:C:201:TYR:CD1	1:C:242:VAL:HG22	2.56	0.41
1:C:245:ARG:HD3	1:C:249:PHE:CE2	2.55	0.41
1:D:160:LYS:HG3	1:D:162:ASP:OD1	2.20	0.41
1:E:95:HIS:HB2	1:E:131:TYR:CE1	2.56	0.41
1:B:113:CYS:HB3	1:B:238:ILE:HG13	2.03	0.41
1:B:115:GLN:HB2	1:B:120:ILE:HG12	2.03	0.41
1:E:253:LEU:HD13	1:E:294:LEU:HD21	2.03	0.41
1:A:22:LEU:HD23	1:A:22:LEU:HA	1.88	0.40
1:A:204:LEU:HA	1:A:204:LEU:HD23	1.90	0.40
1:A:262:THR:OG1	1:A:301:ASP:OD2	2.30	0.40
1:E:81:ALA:HB1	1:E:89:PHE:CE1	2.56	0.40
1:E:116:SER:O	1:E:120:ILE:HG12	2.21	0.40
1:F:182:GLU:CD	1:F:217:LYS:HD2	2.41	0.40
1:D:32:ASP:OD1	1:D:35:SER:HB2	2.21	0.40
1:E:163:GLU:OE1	1:E:199:ARG:HA	2.20	0.40
1:A:187:THR:HG21	1:A:189:GLU:HG3	2.04	0.40
1:F:307:LYS:HE2	3:F:1181:HOH:O	2.21	0.40
1:B:58:LEU:HD23	1:C:198:THR:HG21	2.02	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	313/315 (99%)	302 (96%)	10 (3%)	1 (0%)	41 32
1	B	313/315 (99%)	303 (97%)	7 (2%)	3 (1%)	15 6
1	C	313/315 (99%)	305 (97%)	8 (3%)	0	100 100
1	D	313/315 (99%)	305 (97%)	8 (3%)	0	100 100
1	E	313/315 (99%)	305 (97%)	8 (3%)	0	100 100
1	F	313/315 (99%)	304 (97%)	8 (3%)	1 (0%)	41 32
All	All	1878/1890 (99%)	1824 (97%)	49 (3%)	5 (0%)	41 32

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	259	GLY
1	B	258	LYS
1	B	259	GLY
1	B	262	THR
1	F	101	LEU

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	260/260 (100%)	238 (92%)	22 (8%)	10 2
1	B	260/260 (100%)	241 (93%)	19 (7%)	14 3
1	C	260/260 (100%)	238 (92%)	22 (8%)	10 2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	260/260 (100%)	235 (90%)	25 (10%)	8 1
1	E	260/260 (100%)	232 (89%)	28 (11%)	6 1
1	F	260/260 (100%)	233 (90%)	27 (10%)	7 1
All	All	1560/1560 (100%)	1417 (91%)	143 (9%)	9 1

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ARG
1	A	24	LYS
1	A	27	LYS
1	A	29	ILE
1	A	34	LYS
1	A	50	GLN
1	A	63	LEU
1	A	72	SER
1	A	80	LEU
1	A	101	LEU
1	A	133	GLU
1	A	203	GLN
1	A	213	LYS
1	A	220	LEU
1	A	262	THR
1	A	265	LYS
1	A	274	ARG
1	A	281	ASN
1	A	287	GLN
1	A	296	GLU
1	A	310	LEU
1	A	313	ILE
1	B	3	VAL
1	B	35	SER
1	B	63	LEU
1	B	80	LEU
1	B	101	LEU
1	B	120	ILE
1	B	132	LYS
1	B	133	GLU
1	B	137	LYS
1	B	199	ARG
1	B	203	GLN

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Mol	Chain	Res	Type
1	B	220	LEU
1	B	245	ARG
1	B	260	LEU
1	B	262	THR
1	B	274	ARG
1	B	297	PHE
1	B	307	LYS
1	B	310	LEU
1	C	23	ARG
1	C	24	LYS
1	C	29	ILE
1	C	63	LEU
1	C	80	LEU
1	C	88	GLU
1	C	101	LEU
1	C	132	LYS
1	C	133	GLU
1	C	134	ASP
1	C	137	LYS
1	C	185	ILE
1	C	196	LEU
1	C	203	GLN
1	C	220	LEU
1	C	258	LYS
1	C	260	LEU
1	C	274	ARG
1	C	297	PHE
1	C	300	ASP
1	C	307	LYS
1	C	310	LEU
1	D	8	LYS
1	D	23	ARG
1	D	27	LYS
1	D	29	ILE
1	D	34	LYS
1	D	50	GLN
1	D	63	LEU
1	D	101	LEU
1	D	128	LYS
1	D	132	LYS
1	D	133	GLU
1	D	134	ASP

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Mol	Chain	Res	Type
1	D	137	LYS
1	D	142	GLU
1	D	185	ILE
1	D	199	ARG
1	D	203	GLN
1	D	216	ASN
1	D	220	LEU
1	D	258	LYS
1	D	262	THR
1	D	274	ARG
1	D	297	PHE
1	D	300	ASP
1	D	310	LEU
1	E	8	LYS
1	E	23	ARG
1	E	24	LYS
1	E	29	ILE
1	E	34	LYS
1	E	63	LEU
1	E	80	LEU
1	E	85	LYS
1	E	101	LEU
1	E	120	ILE
1	E	129	LEU
1	E	133	GLU
1	E	134	ASP
1	E	137	LYS
1	E	179	GLN
1	E	185	ILE
1	E	190	SER
1	E	199	ARG
1	E	203	GLN
1	E	220	LEU
1	E	258	LYS
1	E	260	LEU
1	E	265	LYS
1	E	292	LYS
1	E	297	PHE
1	E	302	CYS
1	E	307	LYS
1	E	310	LEU
1	F	23	ARG

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Mol	Chain	Res	Type
1	F	24	LYS
1	F	29	ILE
1	F	63	LEU
1	F	80	LEU
1	F	99	LYS
1	F	101	LEU
1	F	128	LYS
1	F	133	GLU
1	F	134	ASP
1	F	137	LYS
1	F	185	ILE
1	F	196	LEU
1	F	199	ARG
1	F	203	GLN
1	F	216	ASN
1	F	217	LYS
1	F	220	LEU
1	F	225	ASN
1	F	231	ILE
1	F	245	ARG
1	F	258	LYS
1	F	260	LEU
1	F	274	ARG
1	F	284	GLU
1	F	297	PHE
1	F	300	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	62	HIS
1	A	106	ASN
1	A	169	HIS
1	A	203	GLN
1	A	205	HIS
1	A	233	ASN
1	B	62	HIS
1	B	106	ASN
1	B	148	GLN
1	B	203	GLN
1	B	205	HIS

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Mol	Chain	Res	Type
1	B	216	ASN
1	B	233	ASN
1	C	106	ASN
1	C	169	HIS
1	C	203	GLN
1	C	205	HIS
1	C	233	ASN
1	C	287	GLN
1	D	10	HIS
1	D	50	GLN
1	D	62	HIS
1	D	106	ASN
1	D	179	GLN
1	D	203	GLN
1	D	205	HIS
1	D	216	ASN
1	D	233	ASN
1	E	62	HIS
1	E	106	ASN
1	E	121	HIS
1	E	148	GLN
1	E	179	GLN
1	E	203	GLN
1	E	205	HIS
1	E	216	ASN
1	E	233	ASN
1	E	287	GLN
1	F	10	HIS
1	F	106	ASN
1	F	203	GLN
1	F	205	HIS
1	F	216	ASN
1	F	233	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 11 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	315/315 (100%)	0.10	7 (2%) 62 69	19, 30, 59, 158	0
1	B	315/315 (100%)	0.07	10 (3%) 47 55	11, 27, 58, 158	0
1	C	315/315 (100%)	0.04	6 (1%) 66 72	12, 25, 59, 158	0
1	D	315/315 (100%)	0.09	11 (3%) 44 51	12, 26, 62, 158	0
1	E	315/315 (100%)	0.14	5 (1%) 72 77	16, 33, 63, 156	0
1	F	315/315 (100%)	0.06	7 (2%) 62 69	12, 28, 61, 158	0
All	All	1890/1890 (100%)	0.08	46 (2%) 59 66	11, 28, 62, 158	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	260	LEU	18.5
1	B	260	LEU	16.0
1	F	260	LEU	15.2
1	C	259	GLY	12.8
1	C	261	GLY	11.2
1	E	260	LEU	11.1
1	A	260	LEU	9.2
1	D	260	LEU	8.5
1	C	29	ILE	7.8
1	D	259	GLY	6.8
1	C	262	THR	5.7
1	A	259	GLY	5.1
1	B	259	GLY	5.1
1	D	262	THR	4.6
1	C	28	GLY	4.6
1	B	29	ILE	4.6
1	E	262	THR	4.5
1	A	261	GLY	4.3
1	E	259	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
1	E	261	GLY	3.8
1	F	29	ILE	3.7
1	F	259	GLY	3.6
1	F	261	GLY	3.6
1	A	262	THR	3.6
1	B	262	THR	3.5
1	A	29	ILE	3.3
1	E	29	ILE	3.3
1	B	103	THR	3.1
1	B	258	LYS	3.1
1	F	185	ILE	3.0
1	B	261	GLY	3.0
1	B	28	GLY	2.8
1	D	258	LYS	2.7
1	D	101	LEU	2.6
1	D	29	ILE	2.6
1	D	292	LYS	2.5
1	D	261	GLY	2.5
1	D	27	LYS	2.5
1	F	258	LYS	2.4
1	F	216	ASN	2.4
1	D	295	TYR	2.4
1	A	11	ALA	2.2
1	B	185	ILE	2.1
1	D	316	HIS	2.1
1	A	265	LYS	2.0
1	B	101	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CA	E	1125	1/1	0.05	0.50	89,89,89,89	1
2	CA	D	1124	1/1	0.43	0.30	49,49,49,49	1
2	CA	A	1131	1/1	0.81	0.10	60,60,60,60	0
2	CA	C	1133	1/1	0.81	0.10	44,44,44,44	0
2	CA	B	1132	1/1	0.85	0.13	66,66,66,66	0
2	CA	B	1122	1/1	0.87	0.25	59,59,59,59	1
2	CA	A	1121	1/1	0.89	0.16	68,68,68,68	1
2	CA	F	1126	1/1	0.92	0.07	40,40,40,40	1
2	CA	E	1135	1/1	0.95	0.08	54,54,54,54	0
2	CA	D	1134	1/1	0.97	0.06	35,35,35,35	0
2	CA	C	1123	1/1	0.97	0.06	30,30,30,30	1

6.5 Other polymers (i)

There are no such residues in this entry.