Full wwPDB X-ray Structure Validation Report (i)

Sep 28, 2024 – 12:00 PM EDT

PDB ID	:	4QNN
Title	:	Crystal Structure of phospholipase A 1 from hornet(Vespa basalis) venom
Authors	:	Chuang, C.Y.; Ko, T.P.; Wang, A.H.J.; Hou, M.H.
Deposited on	:	2014-06-18
Resolution	:	2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

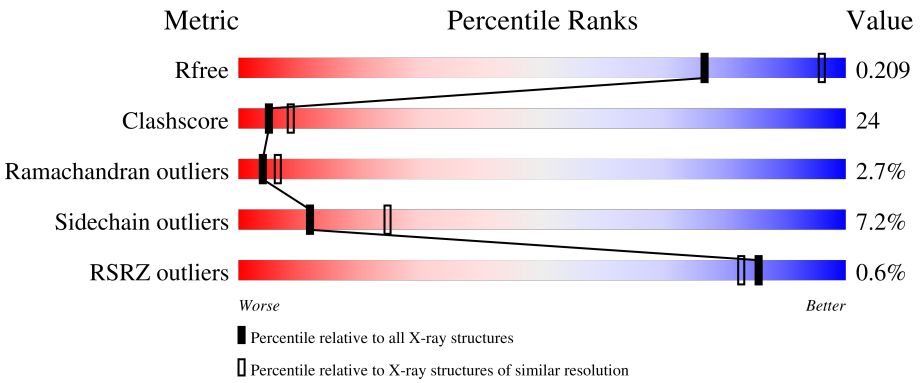
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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	300	% 63% 30% • ••
1	B	300	% 58% 36% 5% ••
1	C	300	63% 30% 5% ••
1	D	300	% 60% 34% • ••

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	CL	A	402	-	-	X	-
2	CL	B	402	-	-	X	-
2	CL	B	403	-	-	X	-
2	CL	B	404	-	-	X	-
2	CL	B	407	-	-	X	-
2	CL	B	410	-	-	X	-
2	CL	B	412	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9672 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 Phospholipase A 1 from hornet(Vespa basalis) venom.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	297	2292	1453	391	429	19	0	0	0
1	B	297	2292	1453	391	429	19	0	0	0
1	C	297	2292	1453	391	429	19	0	0	0
1	D	297	2292	1453	391	429	19	0	0	0

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
2	A	5	5	5	0	0
2	B	12	12	12	0	0
2	C	4	4	4	0	0
2	D	3	3	3	0	0

- Molecule 3 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Hg		
3	A	1	1	1	0	0
3	B	1	1	1	0	0
3	C	1	1	1	0	0

- Molecule 4 is water.

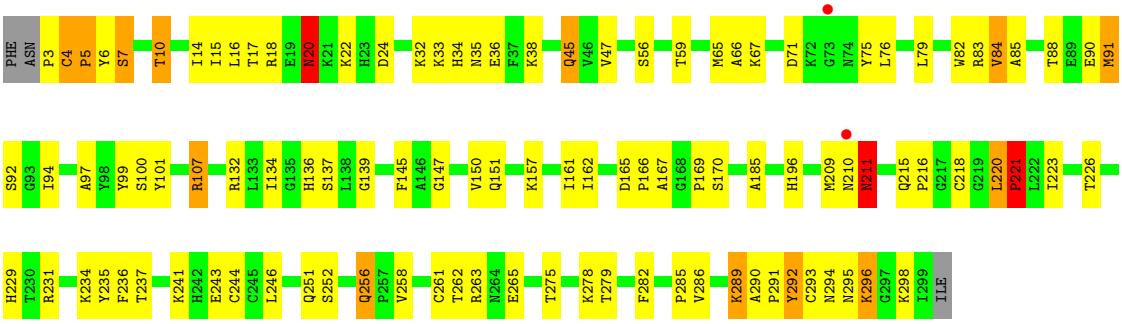
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	120	120	120	0	0
			Total	O		
4	B	112	112	112	0	0
			Total	O		
4	C	117	117	117	0	0
			Total	O		
4	D	128	128	128	0	0

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.

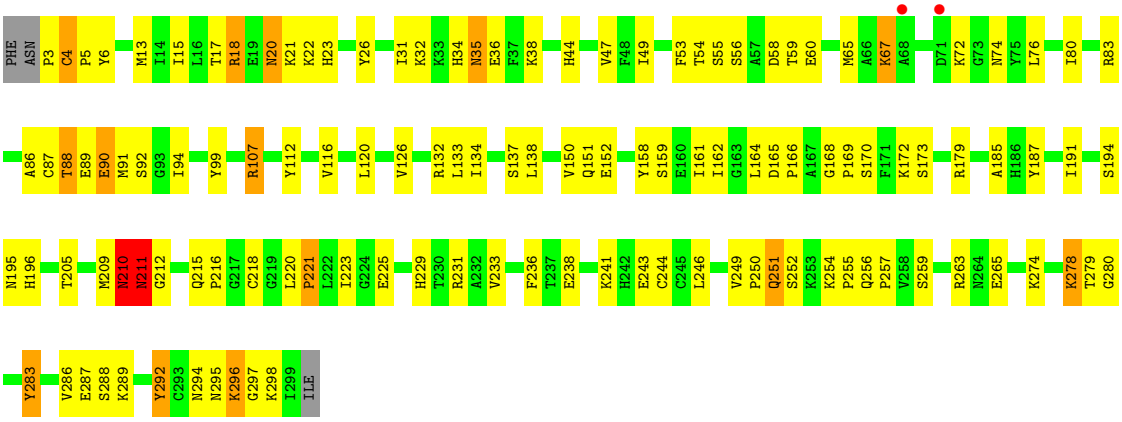
• Molecule 1: Phospholipase A 1 from hornet(Vespa basalis) venom

Chain A:



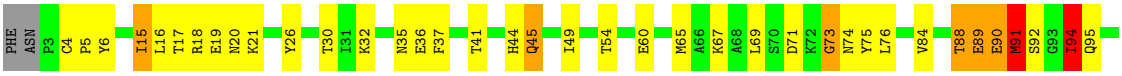
• Molecule 1: Phospholipase A 1 from hornet(Vespa basalis) venom

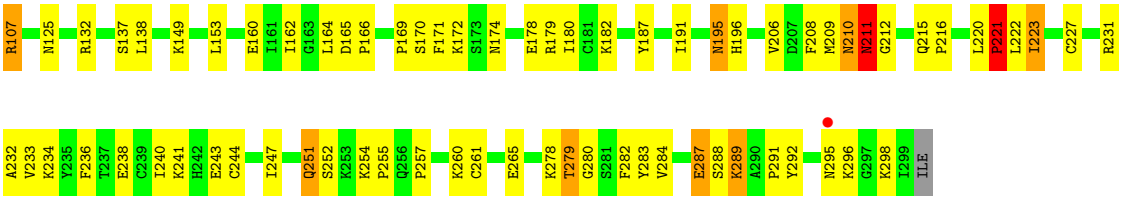
Chain B:



• Molecule 1: Phospholipase A 1 from hornet(Vespa basalis) venom

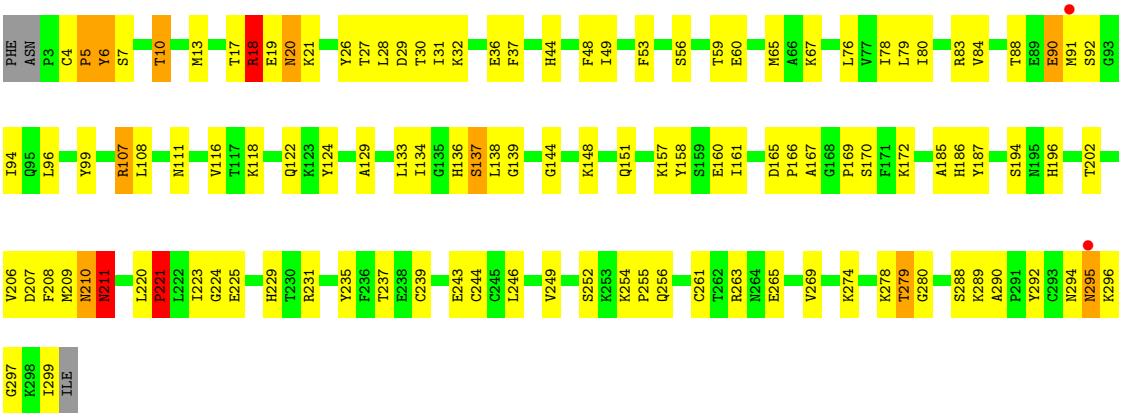
Chain C:





• Molecule 1: Phospholipase A 1 from hornet(Vespa basalis) venom

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	57.28Å 70.15Å 81.72Å 107.14° 109.99° 100.90°	Depositor
Resolution (Å)	25.00 – 2.50 25.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.50) 93.6 (25.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 2.48Å)	Xtriage
Refinement program	REFMAC, CNS 1.1	Depositor
R, R_{free}	0.204 , 0.279 0.208 , 0.209	Depositor DCC
R_{free} test set	1767 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	34.4	Xtriage
Anisotropy	0.422	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 53.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9672	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.88% 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: CL, HG

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	0.65	0/2341	0.82	1/3166 (0.0%)
1	B	0.66	1/2341 (0.0%)	0.84	0/3166
1	C	0.64	0/2341	0.86	1/3166 (0.0%)
1	D	0.65	0/2341	0.83	0/3166
All	All	0.65	1/9364 (0.0%)	0.84	2/12664 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	C	0	1
1	D	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	210	ASN	CB-CG	5.08	1.62	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	45	GLN	N-CA-C	-5.81	95.30	111.00
1	C	73	GLY	N-CA-C	5.44	126.70	113.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	283	TYR	Sidechain
1	B	6	TYR	Sidechain
1	C	6	TYR	Sidechain
1	D	6	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2292	0	2289	112	0
1	B	2292	0	2289	129	0
1	C	2292	0	2289	104	0
1	D	2292	0	2289	111	0
2	A	5	0	0	5	0
2	B	12	0	0	19	0
2	C	4	0	0	1	0
2	D	3	0	0	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	120	0	0	9	0
4	B	112	0	0	5	0
4	C	117	0	0	5	0
4	D	128	0	0	12	0
All	All	9672	0	9156	449	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 24.

All (449) 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:A:209:MET:SD	1:A:209:MET:CE	2.04	1.45
1:B:251:GLN:HE21	1:B:251:GLN:HA	0.98	1.13
1:C:17:THR:HG21	1:C:36:GLU:HG3	1.33	1.10
1:B:107:ARG:HH11	1:B:107:ARG:HB3	1.16	1.08
1:D:18:ARG:HG2	1:D:18:ARG:HH11	1.15	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ARG:HH22	1:B:297:GLY:HA3	1.16	1.07
1:B:251:GLN:HE22	1:B:283:TYR:HB2	1.20	1.02
1:C:251:GLN:HE21	1:C:251:GLN:HA	1.25	0.99
4:A:577:HOH:O	2:B:402:CL:CL	2.18	0.98
1:A:65:MET:HE1	1:A:134:ILE:HG21	1.49	0.95
1:A:298:LYS:NZ	2:A:402:CL:CL	2.37	0.94
1:B:251:GLN:HA	1:B:251:GLN:NE2	1.82	0.94
1:B:56:SER:O	1:B:59:THR:HG23	1.67	0.94
1:B:107:ARG:HB3	1:B:107:ARG:NH1	1.84	0.93
2:B:401:CL:CL	4:C:682:HOH:O	2.25	0.92
1:B:72:LYS:NZ	2:B:407:CL:CL	2.41	0.91
1:B:35:ASN:HA	1:B:38:LYS:HE2	1.50	0.90
1:B:278:LYS:HD3	1:B:279:THR:H	1.34	0.90
1:B:241:LYS:HD3	2:B:404:CL:CL	2.09	0.90
1:C:15:ILE:HG22	1:C:76:LEU:HD11	1.52	0.90
1:C:251:GLN:HE21	1:C:251:GLN:CA	1.85	0.89
1:B:279:THR:HG22	4:B:564:HOH:O	1.73	0.89
1:D:65:MET:HE1	1:D:134:ILE:HG21	1.53	0.89
1:A:211:ASN:N	1:A:211:ASN:HD22	1.68	0.89
1:B:298:LYS:NZ	2:B:412:CL:CL	2.44	0.87
1:A:220:LEU:HB2	1:A:223:ILE:CG2	2.05	0.86
1:D:7:SER:HB3	1:D:10:THR:OG1	1.75	0.86
1:B:278:LYS:HD3	1:B:279:THR:N	1.90	0.85
1:B:251:GLN:HE21	1:B:251:GLN:CA	1.83	0.84
1:D:107:ARG:H	1:D:107:ARG:HD2	1.43	0.83
1:A:20:ASN:HD21	1:A:35:ASN:ND2	1.76	0.83
1:B:220:LEU:HB2	1:B:223:ILE:CG2	2.08	0.83
1:D:211:ASN:HD22	1:D:211:ASN:N	1.76	0.83
1:A:17:THR:HG21	1:A:36:GLU:HG3	1.58	0.83
1:A:18:ARG:NH2	1:B:297:GLY:HA3	1.92	0.83
1:C:211:ASN:N	1:C:211:ASN:HD22	1.75	0.83
1:C:251:GLN:HA	1:C:251:GLN:NE2	1.91	0.83
1:B:72:LYS:HD3	2:B:407:CL:CL	2.14	0.83
1:B:251:GLN:NE2	1:B:283:TYR:HB2	1.93	0.82
1:A:56:SER:O	1:A:59:THR:HG23	1.80	0.82
1:C:195:ASN:H	1:C:195:ASN:HD22	1.27	0.82
1:C:107:ARG:HB3	1:C:107:ARG:HH11	1.43	0.82
1:B:107:ARG:HH11	1:B:107:ARG:CB	1.93	0.81
1:B:211:ASN:N	1:B:211:ASN:HD22	1.75	0.81
1:D:18:ARG:HG2	1:D:18:ARG:NH1	1.86	0.81
1:A:256:GLN:H	1:A:256:GLN:NE2	1.78	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:LYS:CE	2:B:407:CL:CL	2.66	0.81
1:A:220:LEU:HB2	1:A:223:ILE:HG22	1.65	0.79
1:B:17:THR:HG21	1:B:36:GLU:HG3	1.64	0.79
1:C:18:ARG:HG3	1:C:19:GLU:OE2	1.83	0.78
1:A:211:ASN:O	4:A:525:HOH:O	2.00	0.78
1:B:210:ASN:C	1:B:211:ASN:HD22	1.87	0.77
1:C:107:ARG:HB3	1:C:107:ARG:NH1	1.99	0.77
1:D:56:SER:O	1:D:59:THR:HG23	1.86	0.76
1:A:295:ASN:O	4:A:576:HOH:O	2.02	0.76
1:C:210:ASN:C	1:C:211:ASN:HD22	1.89	0.76
1:A:256:GLN:HG3	4:A:565:HOH:O	1.85	0.76
1:C:17:THR:HG22	1:C:76:LEU:HD13	1.68	0.76
1:C:257:PRO:HG2	1:C:260:LYS:HG3	1.68	0.76
1:B:35:ASN:H	1:B:35:ASN:ND2	1.85	0.74
1:C:220:LEU:HB2	1:C:223:ILE:CG2	2.17	0.74
2:B:412:CL:CL	4:C:682:HOH:O	2.42	0.74
1:C:187:TYR:OH	1:C:206:VAL:HG21	1.87	0.74
1:B:210:ASN:H	1:B:210:ASN:HD22	1.35	0.73
1:B:287:GLU:HB2	1:B:292:TYR:HA	1.70	0.73
1:B:220:LEU:HB2	1:B:223:ILE:HG22	1.70	0.73
1:A:10:THR:HG21	1:A:84:VAL:HG21	1.71	0.73
1:D:210:ASN:N	1:D:210:ASN:HD22	1.86	0.73
2:A:402:CL:CL	2:B:407:CL:CL	2.80	0.72
1:C:94:ILE:HD13	1:C:94:ILE:H	1.53	0.72
1:A:210:ASN:C	1:A:211:ASN:HD22	1.92	0.72
1:C:15:ILE:CG2	1:C:76:LEU:HD11	2.19	0.72
1:A:20:ASN:ND2	1:A:35:ASN:HD22	1.88	0.71
1:A:20:ASN:HD21	1:A:35:ASN:HD22	1.38	0.71
1:D:21:LYS:HZ3	1:D:67:LYS:HZ2	1.39	0.71
1:A:18:ARG:HH22	1:B:297:GLY:CA	1.98	0.71
1:A:221:PRO:O	4:A:540:HOH:O	2.09	0.70
1:C:162:ILE:HD13	1:C:236:PHE:CZ	2.27	0.70
1:B:72:LYS:CD	2:B:407:CL:CL	2.76	0.69
1:B:231:ARG:NH2	1:D:60:GLU:OE1	2.25	0.69
1:B:89:GLU:O	1:B:90:GLU:HB3	1.91	0.69
1:D:210:ASN:HD22	1:D:210:ASN:H	1.40	0.69
1:D:202:THR:HG22	4:D:603:HOH:O	1.91	0.69
1:A:210:ASN:C	1:A:211:ASN:ND2	2.46	0.69
1:A:220:LEU:HB2	1:A:223:ILE:HG21	1.74	0.68
4:C:650:HOH:O	2:D:401:CL:CL	2.48	0.68
1:D:118:LYS:O	1:D:122:GLN:HG3	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:408:CL:CL	2:B:411:CL:CL	2.85	0.68
1:D:17:THR:HG21	1:D:36:GLU:HG3	1.75	0.68
1:C:251:GLN:HE21	1:C:252:SER:N	1.90	0.68
1:D:17:THR:CG2	1:D:76:LEU:HD12	2.25	0.67
1:B:22:LYS:NZ	1:B:35:ASN:HD21	1.93	0.67
1:C:17:THR:CG2	1:C:76:LEU:HD13	2.25	0.66
1:C:220:LEU:HB2	1:C:223:ILE:HG22	1.76	0.66
1:D:295:ASN:OD1	1:D:297:GLY:N	2.27	0.66
1:A:296:LYS:HD2	1:A:296:LYS:N	2.11	0.66
1:D:65:MET:HE1	1:D:134:ILE:CG2	2.24	0.66
1:B:252:SER:O	1:B:255:PRO:HD3	1.97	0.65
1:C:15:ILE:HG21	1:C:37:PHE:HE2	1.62	0.65
1:B:90:GLU:O	1:B:92:SER:N	2.30	0.65
1:A:17:THR:OG1	1:A:20:ASN:HB2	1.97	0.64
1:C:107:ARG:HH11	1:C:107:ARG:CB	2.10	0.64
1:B:17:THR:OG1	1:B:20:ASN:HB2	1.96	0.64
1:A:22:LYS:HB3	1:A:24:ASP:OD2	1.96	0.64
1:A:20:ASN:OD1	1:A:22:LYS:HE2	1.98	0.64
1:A:211:ASN:N	1:A:211:ASN:ND2	2.42	0.64
1:D:202:THR:HG23	1:D:207:ASP:OD2	1.97	0.64
1:B:162:ILE:HD13	1:B:236:PHE:CZ	2.34	0.63
1:B:220:LEU:HB2	1:B:223:ILE:HG21	1.81	0.63
1:D:224:GLY:HA2	4:D:531:HOH:O	1.98	0.63
1:A:161:ILE:HG13	1:A:185:ALA:HB2	1.81	0.63
1:C:251:GLN:HE21	1:C:252:SER:H	1.44	0.63
1:A:17:THR:CG2	1:A:36:GLU:HG3	2.28	0.63
1:B:295:ASN:OD1	1:B:297:GLY:N	2.23	0.63
1:C:252:SER:O	1:C:255:PRO:HD3	1.99	0.62
1:B:274:LYS:HG2	4:B:578:HOH:O	2.00	0.62
1:D:107:ARG:H	1:D:107:ARG:CD	2.13	0.62
1:A:65:MET:HE1	1:A:134:ILE:CG2	2.29	0.61
2:B:404:CL:CL	2:B:410:CL:CL	2.92	0.61
1:B:215:GLN:O	1:B:218:CYS:HB2	1.99	0.61
1:C:21:LYS:O	1:C:21:LYS:HG2	2.01	0.61
1:A:231:ARG:HD2	1:A:235:TYR:CE1	2.35	0.61
1:B:179:ARG:HG3	1:B:179:ARG:HH11	1.64	0.61
1:A:20:ASN:ND2	1:A:35:ASN:ND2	2.45	0.61
1:C:210:ASN:C	1:C:211:ASN:ND2	2.53	0.61
1:B:210:ASN:C	1:B:211:ASN:ND2	2.53	0.61
1:A:151:GLN:OE1	1:A:157:LYS:HE2	2.01	0.61
1:C:17:THR:HG21	1:C:36:GLU:CG	2.21	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:LEU:O	1:B:126:VAL:HG23	2.01	0.61
1:C:220:LEU:HD22	1:C:221:PRO:HD2	1.83	0.60
1:D:211:ASN:O	4:D:563:HOH:O	2.17	0.60
1:C:251:GLN:NE2	1:C:252:SER:H	1.99	0.60
1:C:238:GLU:OE1	1:C:241:LYS:HD2	2.02	0.60
1:D:256:GLN:H	1:D:256:GLN:CD	2.06	0.59
1:B:210:ASN:H	1:B:210:ASN:ND2	2.00	0.59
1:B:18:ARG:HG3	1:B:18:ARG:HH11	1.66	0.59
1:A:215:GLN:O	1:A:218:CYS:HB2	2.03	0.59
1:B:54:THR:C	1:B:88:THR:HG23	2.23	0.59
1:A:209:MET:C	1:A:211:ASN:H	2.06	0.59
1:D:220:LEU:HB2	1:D:223:ILE:HG22	1.84	0.59
1:D:21:LYS:NZ	1:D:67:LYS:NZ	2.50	0.59
1:B:22:LYS:HZ2	1:B:35:ASN:HD21	1.50	0.58
1:D:18:ARG:HH11	1:D:18:ARG:CG	2.03	0.58
1:D:137:SER:OG	1:D:138:LEU:N	2.36	0.58
1:D:210:ASN:C	1:D:211:ASN:ND2	2.56	0.58
1:D:21:LYS:NZ	1:D:67:LYS:HZ2	2.01	0.58
1:B:279:THR:CG2	4:B:564:HOH:O	2.41	0.58
1:B:295:ASN:OD1	1:B:296:LYS:N	2.37	0.58
1:A:278:LYS:HD2	1:A:282:PHE:CZ	2.38	0.58
1:D:53:PHE:CE1	1:D:99:TYR:HA	2.38	0.58
1:B:205:THR:O	1:B:279:THR:HG23	2.03	0.58
1:D:211:ASN:N	1:D:211:ASN:ND2	2.47	0.57
1:D:210:ASN:C	1:D:211:ASN:HD22	2.07	0.57
1:B:60:GLU:HG3	1:D:289:LYS:HA	1.86	0.57
1:C:179:ARG:HG3	1:C:180:ILE:O	2.04	0.57
1:C:89:GLU:O	1:C:90:GLU:HB3	2.04	0.57
1:D:17:THR:HG22	1:D:76:LEU:HD12	1.84	0.57
1:A:18:ARG:NH1	1:B:298:LYS:H	2.02	0.57
1:D:107:ARG:HD2	1:D:107:ARG:N	2.15	0.57
1:C:220:LEU:CB	1:C:223:ILE:HG22	2.34	0.57
1:C:210:ASN:H	1:C:210:ASN:ND2	2.03	0.56
1:C:211:ASN:N	1:C:211:ASN:ND2	2.50	0.56
1:A:209:MET:C	1:A:211:ASN:N	2.58	0.56
1:B:169:PRO:O	1:B:170:SER:HB2	2.04	0.56
1:B:4:CYS:SG	1:B:4:CYS:O	2.64	0.56
1:B:17:THR:CG2	1:B:36:GLU:HG3	2.35	0.56
1:B:246:LEU:HD21	1:B:286:VAL:HG12	1.87	0.56
1:C:91:MET:HE1	1:C:95:GLN:HA	1.87	0.56
1:D:31:ILE:HG23	1:D:32:LYS:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:PRO:O	1:D:170:SER:HB2	2.05	0.56
1:D:90:GLU:O	1:D:92:SER:N	2.39	0.56
1:C:90:GLU:O	1:C:92:SER:N	2.39	0.56
1:D:79:LEU:HD12	1:D:79:LEU:N	2.19	0.56
1:C:279:THR:CG2	1:C:280:GLY:N	2.69	0.56
1:A:18:ARG:HH12	1:B:298:LYS:H	1.54	0.55
1:C:17:THR:OG1	1:C:20:ASN:HB2	2.05	0.55
1:D:196:HIS:NE2	4:D:623:HOH:O	2.12	0.55
1:A:17:THR:HG23	1:A:76:LEU:HD12	1.86	0.55
1:A:296:LYS:HE3	4:A:566:HOH:O	2.07	0.55
1:B:18:ARG:HG3	1:B:18:ARG:NH1	2.20	0.55
1:B:243:GLU:O	1:B:244:CYS:HB2	2.06	0.55
1:A:4:CYS:N	1:A:5:PRO:HD3	2.21	0.55
1:B:263:ARG:HH11	1:B:263:ARG:HG3	1.71	0.55
1:C:164:LEU:HD13	1:C:233:VAL:HA	1.88	0.55
1:C:279:THR:HG23	1:C:280:GLY:N	2.22	0.54
1:D:243:GLU:HA	4:D:577:HOH:O	2.06	0.54
1:C:261:CYS:O	1:D:18:ARG:NH2	2.41	0.54
1:A:256:GLN:H	1:A:256:GLN:CD	2.06	0.54
1:C:15:ILE:HG22	1:C:76:LEU:CD1	2.30	0.54
1:D:10:THR:HB	4:D:518:HOH:O	2.07	0.54
1:D:111:ASN:HB3	4:D:517:HOH:O	2.08	0.54
1:A:4:CYS:N	1:A:5:PRO:CD	2.71	0.54
1:B:44:HIS:HA	1:B:74:ASN:ND2	2.23	0.54
2:B:402:CL:CL	2:B:407:CL:CL	3.00	0.53
1:A:162:ILE:HD13	1:A:236:PHE:CZ	2.42	0.53
1:D:256:GLN:H	1:D:256:GLN:NE2	2.06	0.53
1:A:296:LYS:N	1:A:296:LYS:CD	2.71	0.53
1:C:69:LEU:CD2	1:C:240:ILE:HD13	2.39	0.53
1:C:216:PRO:O	1:C:231:ARG:NH2	2.29	0.53
1:D:26:TYR:HE2	4:D:590:HOH:O	1.90	0.53
1:C:20:ASN:HD21	1:C:35:ASN:HD22	1.57	0.53
1:C:169:PRO:O	1:C:170:SER:HB2	2.09	0.53
1:D:220:LEU:HB3	1:D:221:PRO:HD2	1.91	0.53
1:D:299:ILE:C	4:D:628:HOH:O	2.47	0.53
2:A:402:CL:CL	2:B:402:CL:CL	3.01	0.52
1:B:246:LEU:CD2	1:B:286:VAL:HG12	2.39	0.52
1:C:26:TYR:HD1	1:C:30:THR:O	1.92	0.52
1:C:45:GLN:CA	1:C:45:GLN:HE21	2.20	0.52
1:A:234:LYS:HE2	1:A:292:TYR:OH	2.10	0.52
1:C:94:ILE:HD13	1:C:94:ILE:N	2.20	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:ILE:C	1:A:16:LEU:HD23	2.30	0.52
1:B:35:ASN:HA	1:B:38:LYS:CE	2.33	0.52
1:C:220:LEU:HB2	1:C:223:ILE:HG21	1.92	0.52
1:A:97:ALA:O	1:A:100:SER:HB3	2.09	0.52
1:B:35:ASN:CA	1:B:38:LYS:HE2	2.33	0.52
1:C:257:PRO:CG	1:C:260:LYS:HG3	2.39	0.52
1:C:49:ILE:HD13	1:C:65:MET:HE2	1.92	0.52
1:C:257:PRO:HG2	1:C:260:LYS:CG	2.39	0.51
1:A:246:LEU:HD21	1:A:286:VAL:HG12	1.92	0.51
1:B:161:ILE:HG13	1:B:185:ALA:HB2	1.93	0.51
1:B:279:THR:CG2	1:B:280:GLY:N	2.74	0.51
1:C:223:ILE:O	1:C:223:ILE:HD12	2.11	0.51
1:A:18:ARG:HG3	1:A:18:ARG:HH11	1.76	0.51
1:A:220:LEU:CB	1:A:223:ILE:HG22	2.39	0.51
1:D:294:ASN:O	1:D:295:ASN:HB2	2.09	0.51
1:B:65:MET:CE	1:B:134:ILE:HG21	2.41	0.51
1:B:211:ASN:N	1:B:211:ASN:ND2	2.50	0.51
1:B:179:ARG:HG3	1:B:179:ARG:NH1	2.25	0.50
1:B:86:ALA:O	1:B:87:CYS:HB2	2.11	0.50
1:A:5:PRO:O	1:A:84:VAL:HG23	2.11	0.50
1:C:45:GLN:HB3	1:C:75:TYR:CD1	2.46	0.50
2:A:401:CL:CL	2:B:402:CL:CL	3.04	0.50
1:B:168:GLY:O	1:B:172:LYS:HG3	2.12	0.50
1:D:210:ASN:N	1:D:210:ASN:ND2	2.55	0.50
1:C:182:LYS:HG2	4:C:630:HOH:O	2.11	0.50
1:A:67:LYS:HE2	1:A:71:ASP:OD1	2.12	0.49
1:C:17:THR:CG2	1:C:36:GLU:HG3	2.23	0.49
1:C:16:LEU:HD22	1:C:21:LYS:HA	1.94	0.49
1:C:94:ILE:H	1:C:94:ILE:CD1	2.25	0.49
1:C:220:LEU:CD2	1:C:221:PRO:HD2	2.42	0.49
1:D:65:MET:HA	1:D:237:THR:HG23	1.92	0.49
1:B:133:LEU:HD11	1:B:158:TYR:CE2	2.47	0.49
1:A:169:PRO:O	1:A:170:SER:HB2	2.11	0.49
1:A:196:HIS:NE2	4:A:501:HOH:O	2.13	0.49
1:A:262:THR:HG1	1:A:265:GLU:CD	2.16	0.49
1:D:49:ILE:HD13	1:D:65:MET:HE2	1.94	0.49
1:A:99:TYR:OH	1:A:167:ALA:HB1	2.13	0.49
2:B:403:CL:CL	2:B:410:CL:CL	3.05	0.49
1:D:21:LYS:HZ1	1:D:67:LYS:HZ3	1.61	0.49
1:A:4:CYS:O	1:A:4:CYS:SG	2.71	0.49
1:B:209:MET:O	1:B:211:ASN:N	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:ASN:HD22	1:C:178:GLU:HB3	1.76	0.49
2:B:406:CL:CL	2:B:409:CL:CL	3.04	0.49
1:A:15:ILE:O	1:A:16:LEU:HD23	2.13	0.49
1:C:298:LYS:NZ	2:C:501:CL:CL	2.74	0.49
1:B:60:GLU:HG3	1:D:288:SER:O	2.13	0.48
1:B:88:THR:HG22	1:D:223:ILE:HD13	1.95	0.48
1:C:251:GLN:HE21	1:C:251:GLN:C	2.15	0.48
1:C:251:GLN:NE2	1:C:252:SER:N	2.57	0.48
1:A:136:HIS:O	1:A:139:GLY:N	2.46	0.48
1:A:162:ILE:HD13	1:A:236:PHE:HZ	1.79	0.48
1:A:209:MET:O	1:A:211:ASN:N	2.35	0.48
1:A:262:THR:OG1	1:A:265:GLU:OE2	2.28	0.48
1:C:289:LYS:HB2	1:C:289:LYS:NZ	2.28	0.48
1:D:263:ARG:HG3	1:D:263:ARG:HH11	1.78	0.48
1:C:69:LEU:HD21	1:C:240:ILE:HD13	1.96	0.48
1:B:279:THR:HG22	1:B:280:GLY:N	2.28	0.48
1:D:129:ALA:HB2	4:D:585:HOH:O	2.14	0.48
1:A:17:THR:HG23	1:A:76:LEU:CD1	2.44	0.48
1:A:32:LYS:HZ3	1:A:38:LYS:HA	1.79	0.48
1:A:33:LYS:NZ	1:A:33:LYS:HB3	2.29	0.48
1:B:195:ASN:ND2	1:B:196:HIS:CE1	2.82	0.47
1:C:206:VAL:HG11	1:C:208:PHE:CZ	2.49	0.47
1:D:84:VAL:HG22	4:D:621:HOH:O	2.13	0.47
1:A:47:VAL:HG22	1:A:132:ARG:HB2	1.94	0.47
1:B:53:PHE:CE1	1:B:99:TYR:HA	2.49	0.47
1:A:241:LYS:HE2	4:C:676:HOH:O	2.12	0.47
1:B:210:ASN:ND2	1:B:210:ASN:N	2.62	0.47
1:B:83:ARG:NH1	1:D:220:LEU:HD21	2.29	0.47
1:C:227:CYS:O	1:C:231:ARG:HG2	2.14	0.47
1:A:101:TYR:OH	4:A:555:HOH:O	2.18	0.47
1:C:41:THR:OG1	1:C:125:ASN:ND2	2.47	0.47
1:D:187:TYR:OH	4:D:583:HOH:O	2.20	0.47
1:A:6:TYR:CG	1:A:7:SER:N	2.83	0.47
1:C:287:GLU:OE1	1:C:287:GLU:HA	2.15	0.47
1:A:298:LYS:CE	2:A:402:CL:CL	3.00	0.47
1:C:165:ASP:N	1:C:166:PRO:HD3	2.30	0.47
1:D:4:CYS:N	1:D:5:PRO:HD3	2.29	0.47
1:A:251:GLN:HE21	1:A:252:SER:N	2.13	0.47
1:A:278:LYS:HD2	1:A:282:PHE:HZ	1.79	0.47
1:C:215:GLN:HB3	1:C:231:ARG:NH1	2.29	0.47
1:B:187:TYR:CD1	1:B:274:LYS:HB3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:LYS:O	1:C:254:LYS:HG3	2.14	0.47
1:D:206:VAL:HG23	1:D:206:VAL:O	2.14	0.47
1:C:49:ILE:HG23	1:C:65:MET:CE	2.45	0.47
1:D:21:LYS:HZ1	1:D:67:LYS:NZ	2.13	0.47
1:B:34:HIS:O	1:B:38:LYS:HG3	2.14	0.46
1:C:265:GLU:O	1:C:278:LYS:HD3	2.15	0.46
1:D:165:ASP:N	1:D:166:PRO:HD3	2.31	0.46
1:D:252:SER:HB2	1:D:255:PRO:HA	1.97	0.46
1:A:251:GLN:HE21	1:A:252:SER:H	1.63	0.46
1:D:157:LYS:HB2	1:D:186:HIS:CE1	2.50	0.46
1:B:49:ILE:HD13	1:B:65:MET:HE2	1.96	0.46
1:B:35:ASN:HA	1:B:38:LYS:HG3	1.97	0.46
1:A:32:LYS:NZ	1:A:38:LYS:HA	2.31	0.46
1:B:4:CYS:N	1:B:5:PRO:HD3	2.31	0.46
1:D:220:LEU:HB2	1:D:223:ILE:CG2	2.45	0.46
1:A:17:THR:HG21	1:A:36:GLU:CG	2.39	0.46
1:A:258:VAL:O	1:A:261:CYS:HB2	2.16	0.46
1:B:294:ASN:O	1:B:295:ASN:HB2	2.16	0.46
1:D:209:MET:C	1:D:211:ASN:H	2.19	0.46
1:D:252:SER:O	1:D:255:PRO:HG3	2.16	0.46
1:D:133:LEU:HD11	1:D:158:TYR:CE2	2.50	0.46
1:B:238:GLU:OE2	2:B:403:CL:CL	2.71	0.46
1:C:67:LYS:NZ	1:C:71:ASP:OD1	2.43	0.46
1:D:161:ILE:HG13	1:D:185:ALA:HB2	1.98	0.46
1:A:90:GLU:O	1:A:91:MET:C	2.55	0.45
1:B:55:SER:OG	1:B:56:SER:N	2.50	0.45
1:B:88:THR:CG2	1:D:223:ILE:HD13	2.46	0.45
1:D:18:ARG:NH1	1:D:18:ARG:CG	2.67	0.45
1:A:15:ILE:HB	1:A:34:HIS:CD2	2.52	0.45
1:C:5:PRO:O	1:C:84:VAL:CG2	2.64	0.45
1:A:18:ARG:NH1	1:B:298:LYS:N	2.64	0.45
1:B:31:ILE:HG23	1:B:32:LYS:N	2.31	0.45
1:A:90:GLU:O	1:A:92:SER:N	2.50	0.45
1:D:243:GLU:O	1:D:244:CYS:HB2	2.16	0.45
1:C:247:ILE:CD1	1:C:295:ASN:HD22	2.28	0.45
1:D:279:THR:CG2	1:D:280:GLY:N	2.79	0.45
1:B:26:TYR:CE2	1:B:34:HIS:HD2	2.35	0.45
1:B:54:THR:HB	1:D:223:ILE:HD11	1.98	0.45
1:D:6:TYR:CD2	1:D:108:LEU:HD13	2.52	0.45
1:D:239:CYS:SG	1:D:246:LEU:HB2	2.57	0.45
1:B:4:CYS:N	1:B:5:PRO:CD	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:ASN:HA	1:C:284:VAL:O	2.17	0.45
1:D:4:CYS:N	1:D:5:PRO:CD	2.79	0.45
1:D:83:ARG:HB2	1:D:88:THR:CB	2.47	0.45
1:B:35:ASN:H	1:B:35:ASN:HD22	1.60	0.44
1:B:60:GLU:OE1	1:D:231:ARG:NH2	2.50	0.44
1:B:241:LYS:NZ	2:B:403:CL:CL	2.61	0.44
1:D:44:HIS:CD2	1:D:44:HIS:H	2.34	0.44
1:D:83:ARG:HB2	1:D:88:THR:HB	1.98	0.44
1:D:136:HIS:O	1:D:139:GLY:N	2.44	0.44
1:B:3:PRO:HD3	4:B:608:HOH:O	2.17	0.44
1:B:49:ILE:HD13	1:B:65:MET:CE	2.47	0.44
1:D:27:THR:C	1:D:29:ASP:H	2.20	0.44
1:A:243:GLU:OE2	4:A:542:HOH:O	2.21	0.44
1:C:206:VAL:HG13	1:C:282:PHE:CE2	2.53	0.44
1:C:4:CYS:N	1:C:5:PRO:CD	2.80	0.44
1:D:151:GLN:OE1	1:D:157:LYS:HE2	2.18	0.44
1:A:165:ASP:N	1:A:166:PRO:HD3	2.31	0.44
1:B:164:LEU:HD13	1:B:233:VAL:HA	2.00	0.44
1:D:209:MET:C	1:D:211:ASN:N	2.71	0.44
1:D:265:GLU:OE1	1:D:265:GLU:N	2.51	0.44
1:A:82:TRP:HE3	1:A:85:ALA:HB3	1.81	0.44
1:A:84:VAL:CG2	1:A:85:ALA:N	2.80	0.44
1:D:44:HIS:CD2	1:D:44:HIS:N	2.85	0.43
1:B:112:TYR:O	1:B:116:VAL:HG23	2.18	0.43
1:B:295:ASN:ND2	4:B:577:HOH:O	2.48	0.43
1:A:18:ARG:HH12	1:B:297:GLY:CA	2.30	0.43
1:D:79:LEU:HD12	1:D:79:LEU:H	1.81	0.43
1:A:32:LYS:O	1:A:32:LYS:HD3	2.18	0.43
1:A:107:ARG:HG3	1:A:145:PHE:CE2	2.54	0.43
1:A:137:SER:HB3	1:A:229:HIS:NE2	2.33	0.43
1:B:3:PRO:O	1:B:3:PRO:HG2	2.18	0.43
1:B:187:TYR:CG	1:B:274:LYS:HB3	2.54	0.43
1:C:149:LYS:O	1:C:153:LEU:HG	2.18	0.43
1:A:256:GLN:H	1:A:256:GLN:HE21	1.62	0.43
1:D:17:THR:HG22	1:D:76:LEU:HA	2.00	0.43
1:B:32:LYS:HB3	1:B:32:LYS:HE2	1.72	0.43
1:A:289:LYS:HA	1:C:60:GLU:HG3	2.01	0.43
1:C:211:ASN:HB2	1:C:212:GLY:HA2	2.01	0.43
1:C:295:ASN:OD1	1:C:296:LYS:N	2.52	0.43
1:B:137:SER:OG	1:B:138:LEU:N	2.50	0.43
1:B:215:GLN:HA	1:B:216:PRO:HD3	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:194:SER:HB2	1:D:225:GLU:OE1	2.19	0.43
1:A:243:GLU:O	1:A:244:CYS:HB2	2.18	0.43
1:A:285:PRO:HG2	1:A:294:ASN:HD22	1.83	0.43
1:B:150:VAL:HG23	1:B:151:GLN:N	2.34	0.43
1:D:19:GLU:O	1:D:20:ASN:CG	2.57	0.43
1:B:22:LYS:NZ	1:B:35:ASN:ND2	2.65	0.42
1:A:6:TYR:CD2	1:A:7:SER:N	2.87	0.42
1:A:107:ARG:HG3	1:A:145:PHE:CD2	2.54	0.42
1:D:99:TYR:OH	1:D:167:ALA:HB1	2.20	0.42
1:A:147:GLY:O	1:A:150:VAL:HG22	2.19	0.42
1:A:66:ALA:HB2	1:A:79:LEU:HD11	2.01	0.42
1:B:289:LYS:HG2	1:D:60:GLU:HG3	2.00	0.42
1:C:195:ASN:H	1:C:195:ASN:ND2	2.06	0.42
1:C:251:GLN:NE2	1:C:283:TYR:HB2	2.34	0.42
1:D:27:THR:C	1:D:29:ASP:N	2.72	0.42
1:D:249:VAL:HG12	1:D:261:CYS:SG	2.59	0.42
1:C:49:ILE:CG2	1:C:65:MET:HE2	2.50	0.42
1:C:196:HIS:CD2	1:C:222:LEU:HD23	2.55	0.42
1:D:26:TYR:HA	1:D:30:THR:OG1	2.19	0.42
1:D:37:PHE:HD1	1:D:124:TYR:CZ	2.38	0.42
1:A:107:ARG:NH2	1:A:145:PHE:CZ	2.88	0.42
1:A:296:LYS:HD2	1:A:296:LYS:H	1.85	0.42
1:B:21:LYS:CD	1:B:67:LYS:HZ1	2.33	0.42
1:C:132:ARG:HG2	1:C:160:GLU:HB3	2.02	0.42
1:B:256:GLN:HB2	1:B:257:PRO:HD2	2.02	0.41
1:C:45:GLN:HB3	1:C:75:TYR:CE1	2.55	0.41
1:D:48:PHE:HA	1:D:78:ILE:O	2.19	0.41
1:B:137:SER:HB3	1:B:229:HIS:NE2	2.35	0.41
1:B:162:ILE:HD13	1:B:236:PHE:CE2	2.55	0.41
1:B:194:SER:HB2	1:B:225:GLU:OE1	2.20	0.41
1:D:28:LEU:HD21	1:D:116:VAL:HG22	2.03	0.41
1:A:14:ILE:CG2	1:A:16:LEU:HD21	2.50	0.41
1:C:44:HIS:H	1:C:44:HIS:CD2	2.38	0.41
1:A:289:LYS:O	1:A:290:ALA:C	2.57	0.41
1:B:15:ILE:CG2	1:B:76:LEU:HD11	2.49	0.41
1:B:31:ILE:CG2	1:B:32:LYS:N	2.83	0.41
1:C:165:ASP:HB2	1:C:232:ALA:HB2	2.02	0.41
1:C:209:MET:O	1:C:211:ASN:N	2.50	0.41
1:A:18:ARG:HH12	1:B:298:LYS:N	2.16	0.41
1:A:162:ILE:HG21	1:A:236:PHE:CZ	2.56	0.41
1:A:220:LEU:HA	1:A:221:PRO:HD3	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:LYS:HD2	1:C:149:LYS:HA	1.89	0.41
1:D:231:ARG:HB3	1:D:235:TYR:CE2	2.54	0.41
1:B:209:MET:C	1:B:211:ASN:N	2.74	0.41
1:C:18:ARG:CG	1:C:19:GLU:OE2	2.63	0.41
1:D:13:MET:HG2	1:D:80:ILE:HD13	2.02	0.41
1:D:289:LYS:O	1:D:290:ALA:C	2.59	0.41
1:B:47:VAL:HG22	1:B:132:ARG:HB2	2.02	0.41
1:C:44:HIS:CD2	1:C:44:HIS:N	2.89	0.41
1:B:165:ASP:N	1:B:166:PRO:HD3	2.36	0.41
1:B:195:ASN:HD21	1:B:196:HIS:CE1	2.37	0.41
1:D:208:PHE:CD2	1:D:269:VAL:HG22	2.56	0.41
1:A:45:GLN:O	1:A:75:TYR:HA	2.21	0.41
1:A:83:ARG:HB2	1:A:88:THR:HB	2.01	0.41
1:A:263:ARG:NH2	1:A:275:THR:O	2.54	0.41
1:C:54:THR:C	1:C:88:THR:HG23	2.42	0.41
1:C:160:GLU:HA	1:C:187:TYR:O	2.20	0.41
1:C:171:PHE:HA	1:C:174:ASN:OD1	2.21	0.41
1:C:243:GLU:O	1:C:244:CYS:HB2	2.21	0.41
1:D:137:SER:HB2	1:D:229:HIS:NE2	2.36	0.41
1:B:15:ILE:HD13	1:B:15:ILE:N	2.35	0.41
1:B:249:VAL:O	1:B:250:PRO:C	2.59	0.41
1:D:279:THR:HG23	1:D:280:GLY:N	2.36	0.41
1:B:210:ASN:O	1:B:212:GLY:HA2	2.21	0.40
1:D:144:GLY:O	1:D:148:LYS:HG3	2.20	0.40
1:D:165:ASP:OD2	1:D:194:SER:OG	2.29	0.40
1:A:3:PRO:O	1:A:4:CYS:HB3	2.20	0.40
1:D:31:ILE:CG2	1:D:32:LYS:N	2.85	0.40
1:D:263:ARG:HG3	1:D:263:ARG:NH1	2.36	0.40
1:B:13:MET:HG2	1:B:80:ILE:HD13	2.03	0.40
1:D:160:GLU:OE2	1:D:274:LYS:NZ	2.46	0.40
1:A:137:SER:HB3	1:A:229:HIS:CE1	2.57	0.40
1:A:215:GLN:HA	1:A:216:PRO:HD3	1.93	0.40
1:B:15:ILE:HB	1:B:34:HIS:NE2	2.36	0.40
1:C:137:SER:OG	1:C:138:LEU:N	2.54	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	295/300 (98%)	264 (90%)	24 (8%)	7 (2%)	5 8
1	B	295/300 (98%)	262 (89%)	26 (9%)	7 (2%)	5 8
1	C	295/300 (98%)	264 (90%)	22 (8%)	9 (3%)	3 5
1	D	295/300 (98%)	265 (90%)	21 (7%)	9 (3%)	3 5
All	All	1180/1200 (98%)	1055 (89%)	93 (8%)	32 (3%)	4 6

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	MET
1	A	94	ILE
1	A	211	ASN
1	B	90	GLU
1	B	91	MET
1	B	94	ILE
1	B	211	ASN
1	C	90	GLU
1	C	94	ILE
1	C	211	ASN
1	D	91	MET
1	D	94	ILE
1	D	211	ASN
1	C	73	GLY
1	C	91	MET
1	A	20	ASN
1	B	221	PRO
1	C	292	TYR
1	D	90	GLU
1	D	292	TYR
1	D	295	ASN
1	A	293	CYS

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Mol	Chain	Res	Type
1	D	18	ARG
1	A	292	TYR
1	B	20	ASN
1	B	292	TYR
1	C	89	GLU
1	C	172	LYS
1	D	221	PRO
1	D	20	ASN
1	A	221	PRO
1	C	221	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	256/260 (98%)	239 (93%)	17 (7%)	14 28
1	B	256/260 (98%)	234 (91%)	22 (9%)	8 18
1	C	256/260 (98%)	235 (92%)	21 (8%)	9 19
1	D	256/260 (98%)	242 (94%)	14 (6%)	18 37
All	All	1024/1040 (98%)	950 (93%)	74 (7%)	12 24

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	CYS
1	A	5	PRO
1	A	7	SER
1	A	10	THR
1	A	20	ASN
1	A	84	VAL
1	A	107	ARG
1	A	211	ASN
1	A	220	LEU
1	A	221	PRO
1	A	226	THR

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Mol	Chain	Res	Type
1	A	237	THR
1	A	256	GLN
1	A	279	THR
1	A	289	LYS
1	A	291	PRO
1	A	296	LYS
1	B	4	CYS
1	B	18	ARG
1	B	23	HIS
1	B	35	ASN
1	B	58	ASP
1	B	67	LYS
1	B	88	THR
1	B	107	ARG
1	B	152	GLU
1	B	159	SER
1	B	173	SER
1	B	191	ILE
1	B	210	ASN
1	B	211	ASN
1	B	221	PRO
1	B	251	GLN
1	B	254	LYS
1	B	259	SER
1	B	265	GLU
1	B	278	LYS
1	B	288	SER
1	B	296	LYS
1	C	15	ILE
1	C	32	LYS
1	C	45	GLN
1	C	74	ASN
1	C	88	THR
1	C	91	MET
1	C	94	ILE
1	C	107	ARG
1	C	191	ILE
1	C	195	ASN
1	C	210	ASN
1	C	211	ASN
1	C	221	PRO
1	C	223	ILE

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Mol	Chain	Res	Type
1	C	234	LYS
1	C	251	GLN
1	C	279	THR
1	C	287	GLU
1	C	288	SER
1	C	289	LYS
1	C	291	PRO
1	D	5	PRO
1	D	10	THR
1	D	18	ARG
1	D	96	LEU
1	D	107	ARG
1	D	137	SER
1	D	172	LYS
1	D	210	ASN
1	D	211	ASN
1	D	221	PRO
1	D	254	LYS
1	D	278	LYS
1	D	279	THR
1	D	296	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	186	HIS
1	A	211	ASN
1	A	214	ASN
1	A	251	GLN
1	A	256	GLN
1	B	34	HIS
1	B	35	ASN
1	B	45	GLN
1	B	196	HIS
1	B	210	ASN
1	B	211	ASN
1	B	214	ASN
1	B	251	GLN
1	B	272	ASN
1	C	20	ASN
1	C	35	ASN

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Mol	Chain	Res	Type
1	C	44	HIS
1	C	45	GLN
1	C	111	ASN
1	C	125	ASN
1	C	130	ASN
1	C	195	ASN
1	C	210	ASN
1	C	211	ASN
1	C	251	GLN
1	D	44	HIS
1	D	45	GLN
1	D	111	ASN
1	D	125	ASN
1	D	186	HIS
1	D	210	ASN
1	D	211	ASN
1	D	214	ASN
1	D	256	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 27 ligands modelled in this entry, 27 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 (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	297/300 (99%)	-0.23	2 (0%)	84	81	20, 34, 62, 73	0
1	B	297/300 (99%)	-0.19	2 (0%)	84	81	18, 34, 63, 73	0
1	C	297/300 (99%)	-0.21	1 (0%)	90	88	19, 35, 63, 73	0
1	D	297/300 (99%)	-0.27	2 (0%)	84	81	20, 34, 63, 74	0
All	All	1188/1200 (99%)	-0.23	7 (0%)	85	83	18, 34, 63, 74	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	210	ASN	2.6
1	B	71	ASP	2.5
1	D	91	MET	2.3
1	B	68	ALA	2.2
1	A	73	GLY	2.1
1	D	295	ASN	2.1
1	C	295	ASN	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, 95th 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	CL	B	407	1/1	0.91	0.10	33,33,33,33	0
2	CL	A	404	1/1	0.92	0.07	48,48,48,48	0
2	CL	A	401	1/1	0.92	0.11	26,26,26,26	0
2	CL	B	412	1/1	0.92	0.13	43,43,43,43	0
2	CL	C	502	1/1	0.92	0.13	27,27,27,27	0
2	CL	C	504	1/1	0.92	0.17	37,37,37,37	0
2	CL	D	401	1/1	0.93	0.10	36,36,36,36	0
2	CL	B	409	1/1	0.94	0.08	36,36,36,36	0
2	CL	B	402	1/1	0.95	0.12	19,19,19,19	0
2	CL	B	405	1/1	0.95	0.16	31,31,31,31	0
2	CL	A	403	1/1	0.95	0.05	31,31,31,31	0
2	CL	A	405	1/1	0.95	0.11	56,56,56,56	0
2	CL	B	404	1/1	0.96	0.07	28,28,28,28	0
2	CL	D	402	1/1	0.96	0.08	38,38,38,38	0
2	CL	D	403	1/1	0.96	0.05	36,36,36,36	0
3	HG	C	505	1/1	0.96	0.08	70,70,70,70	1
2	CL	C	503	1/1	0.97	0.04	38,38,38,38	0
2	CL	B	410	1/1	0.97	0.08	39,39,39,39	0
2	CL	B	411	1/1	0.97	0.13	39,39,39,39	0
2	CL	B	401	1/1	0.97	0.08	22,22,22,22	0
2	CL	C	501	1/1	0.97	0.09	23,23,23,23	0
3	HG	B	413	1/1	0.97	0.05	62,62,62,62	1
2	CL	A	402	1/1	0.97	0.10	25,25,25,25	0
3	HG	A	406	1/1	0.98	0.06	61,61,61,61	1
2	CL	B	408	1/1	0.98	0.15	32,32,32,32	0
2	CL	B	406	1/1	0.98	0.09	28,28,28,28	0
2	CL	B	403	1/1	0.99	0.04	28,28,28,28	0

6.5 Other polymers (i)

There are no such residues in this entry.