Full wwPDB X-ray Structure Validation Report ⓘ

Sep 5, 2023 – 06:38 PM EDT

PDB ID	:	4EJF
Title	:	Allosteric peptides that bind to a caspase zymogen and mediate caspase tetramerization
Authors	:	Murray, J.M.
Deposited on	:	2012-04-06
Resolution	:	2.65 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:

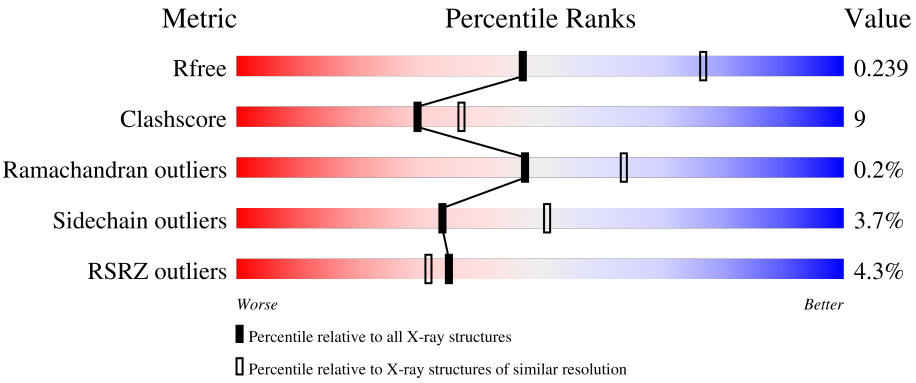
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.65 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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	279	2% 71% 16% 13%
1	B	279	4% 64% 22% · 13%
1	C	279	3% 63% 22% · 13%
1	D	279	4% 69% 18% 13%
2	E	18	11% 50% 11% 6% 33%

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Mol	Chain	Length	Quality of chain
2	F	18	6% 39% 17% 6% 39%
2	G	18	17% 28% 39% 33%
2	H	18	6% 22% 44% 33%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8485 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 Caspase-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	7	0	0
			1947	1243	338	353	13			
1	B	243	Total	C	N	O	S	0	0	0
			1950	1245	338	353	14			
1	C	243	Total	C	N	O	S	0	0	0
			1944	1239	338	353	14			
1	D	243	Total	C	N	O	S	0	0	0
			1950	1245	338	353	14			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	MET	-	expression tag	UNP P55212
A	22	GLY	-	expression tag	UNP P55212
A	23	SER	-	expression tag	UNP P55212
A	163	ALA	CYS	engineered mutation	UNP P55212
A	294	HIS	-	expression tag	UNP P55212
A	295	HIS	-	expression tag	UNP P55212
A	296	HIS	-	expression tag	UNP P55212
A	297	HIS	-	expression tag	UNP P55212
A	298	HIS	-	expression tag	UNP P55212
A	299	HIS	-	expression tag	UNP P55212
B	21	MET	-	expression tag	UNP P55212
B	22	GLY	-	expression tag	UNP P55212
B	23	SER	-	expression tag	UNP P55212
B	163	ALA	CYS	engineered mutation	UNP P55212
B	294	HIS	-	expression tag	UNP P55212
B	295	HIS	-	expression tag	UNP P55212
B	296	HIS	-	expression tag	UNP P55212
B	297	HIS	-	expression tag	UNP P55212
B	298	HIS	-	expression tag	UNP P55212
B	299	HIS	-	expression tag	UNP P55212
C	21	MET	-	expression tag	UNP P55212

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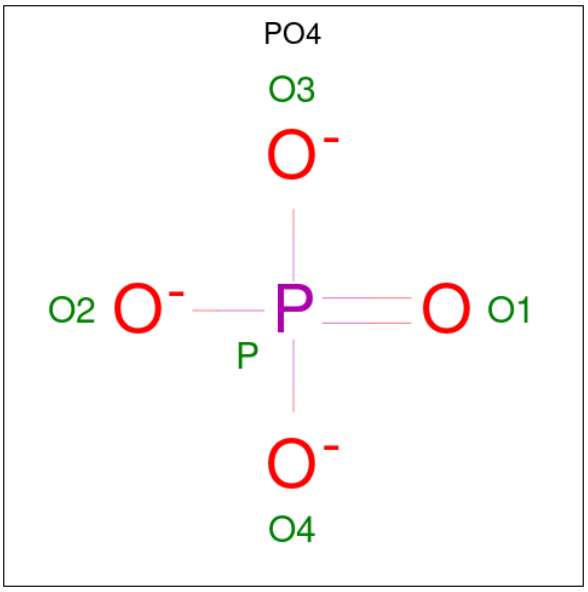
Chain	Residue	Modelled	Actual	Comment	Reference
C	22	GLY	-	expression tag	UNP P55212
C	23	SER	-	expression tag	UNP P55212
C	163	ALA	CYS	engineered mutation	UNP P55212
C	294	HIS	-	expression tag	UNP P55212
C	295	HIS	-	expression tag	UNP P55212
C	296	HIS	-	expression tag	UNP P55212
C	297	HIS	-	expression tag	UNP P55212
C	298	HIS	-	expression tag	UNP P55212
C	299	HIS	-	expression tag	UNP P55212
D	21	MET	-	expression tag	UNP P55212
D	22	GLY	-	expression tag	UNP P55212
D	23	SER	-	expression tag	UNP P55212
D	163	ALA	CYS	engineered mutation	UNP P55212
D	294	HIS	-	expression tag	UNP P55212
D	295	HIS	-	expression tag	UNP P55212
D	296	HIS	-	expression tag	UNP P55212
D	297	HIS	-	expression tag	UNP P55212
D	298	HIS	-	expression tag	UNP P55212
D	299	HIS	-	expression tag	UNP P55212

- Molecule 2 is a protein called phage-derived peptide 419.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	12	Total	C	N	O	S	0	0	0
			102	66	18	17	1			
2	F	11	Total	C	N	O	S	0	0	0
			93	61	17	14	1			
2	G	12	Total	C	N	O	S	0	0	0
			108	69	21	17	1			
2	H	12	Total	C	N	O	S	0	0	0
			102	66	18	17	1			

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0

- Molecule 4 is water.

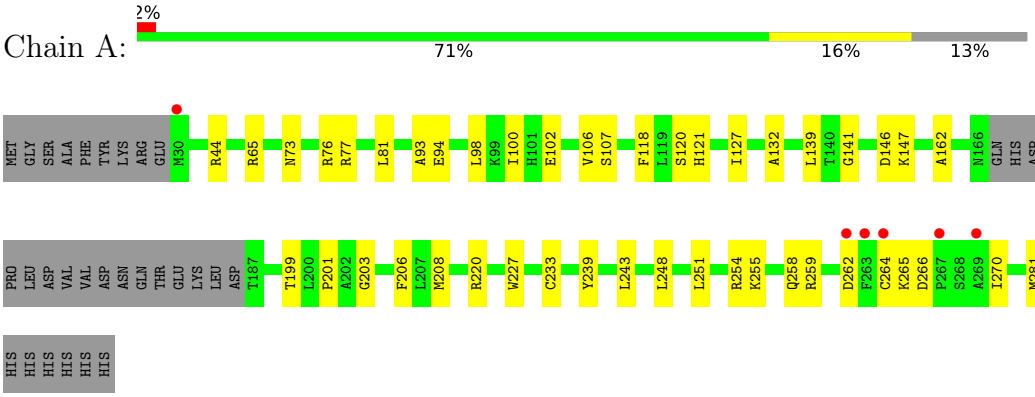
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	65	Total O 65 65	0	0
4	B	72	Total O 72 72	0	0
4	C	61	Total O 61 61	0	0
4	D	74	Total O 74 74	0	0
4	E	2	Total O 2 2	0	0
4	F	3	Total O 3 3	0	0
4	H	2	Total O 2 2	0	0

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.

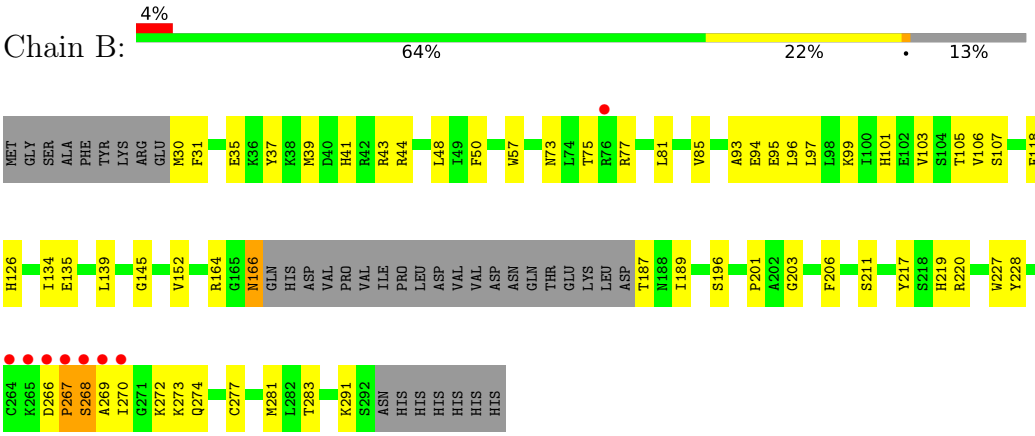
• Molecule 1: Caspase-6

Chain A:



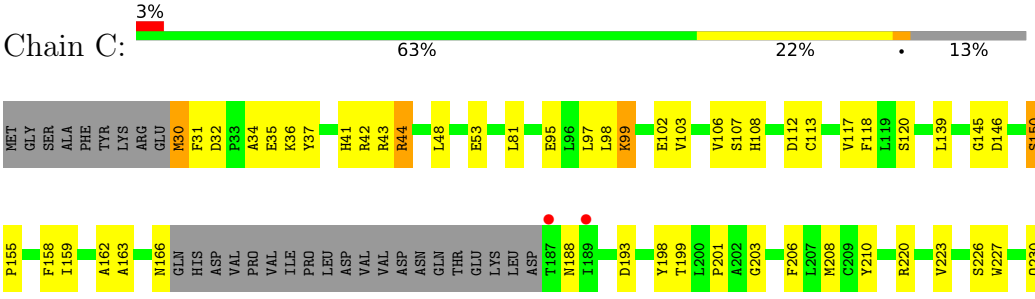
• Molecule 1: Caspase-6

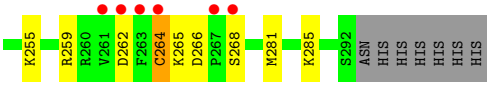
Chain B:



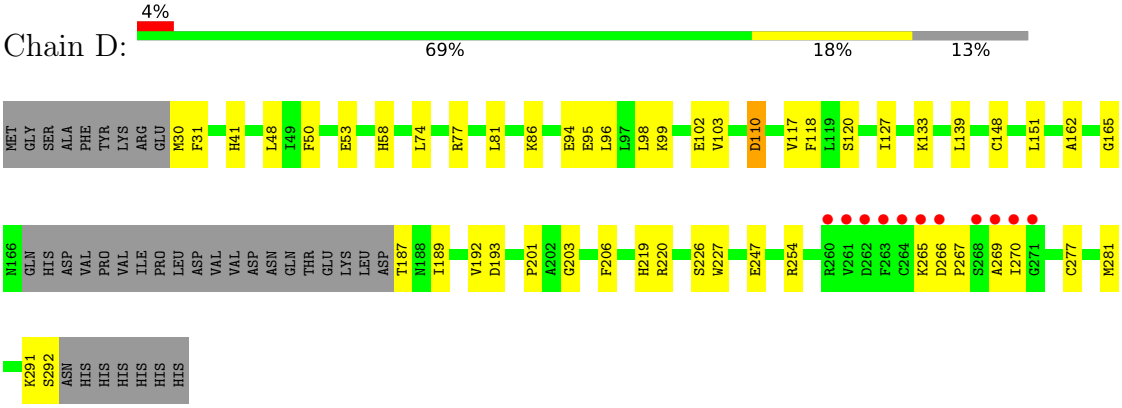
• Molecule 1: Caspase-6

Chain C:

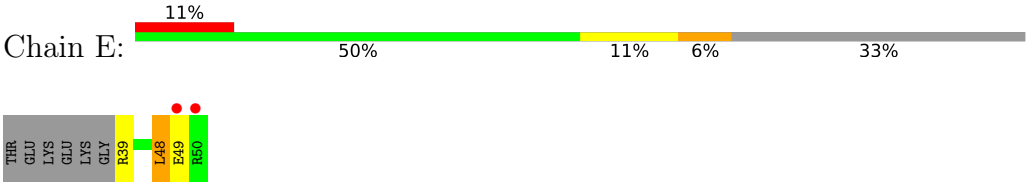




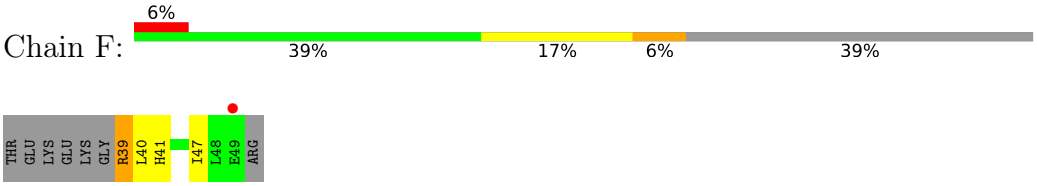
• Molecule 1: Caspase-6



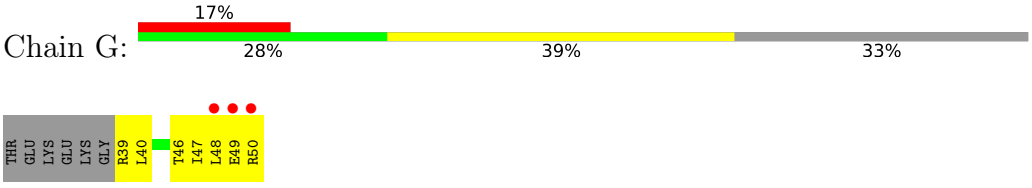
• Molecule 2: phage-derived peptide 419



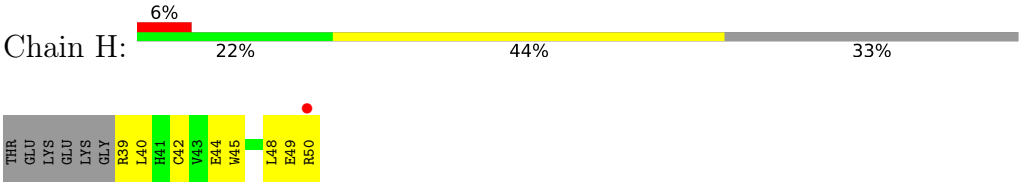
• Molecule 2: phage-derived peptide 419



• Molecule 2: phage-derived peptide 419



• Molecule 2: phage-derived peptide 419



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	128.30Å 105.69Å 91.92Å 90.00° 106.61° 90.00°	Depositor
Resolution (Å)	58.93 – 2.65 80.15 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.4 (58.93-2.65) 92.4 (80.15-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 2.65Å)	Xtriage
Refinement program	PHENIX dev_713	Depositor
R, R_{free}	0.188 , 0.239 0.193 , 0.239	Depositor DCC
R_{free} test set	1720 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	31.4	Xtriage
Anisotropy	0.679	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 50.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8485	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 53.94 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.9251e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.24	0/1992	0.43	0/2683
1	B	0.23	0/1995	0.43	0/2686
1	C	0.25	0/1988	0.41	0/2677
1	D	0.24	0/1995	0.43	1/2686 (0.0%)
2	E	0.22	0/104	0.45	0/141
2	F	0.19	0/95	0.40	0/129
2	G	0.20	0/110	0.42	0/148
2	H	0.22	0/104	0.46	0/141
All	All	0.24	0/8383	0.42	1/11291 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	266	ASP	CB-CG-OD1	-5.53	113.32	118.30

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	1947	0	1915	36	0
1	B	1950	0	1922	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1944	0	1915	42	0
1	D	1950	0	1922	27	0
2	E	102	0	96	1	0
2	F	93	0	90	5	0
2	G	108	0	107	9	0
2	H	102	0	96	11	0
3	C	5	0	0	1	0
3	D	5	0	0	0	0
4	A	65	0	0	0	0
4	B	72	0	0	3	0
4	C	61	0	0	3	0
4	D	74	0	0	0	0
4	E	2	0	0	0	0
4	F	3	0	0	0	0
4	H	2	0	0	0	0
All	All	8485	0	8063	152	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 9.

All (152) 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)
2:G:49:GLU:HG2	2:G:50:ARG:H	1.45	0.81
1:C:30:MET:HG3	1:C:31:PHE:H	1.48	0.79
2:G:50:ARG:C	2:H:39:ARG:HH12	1.86	0.79
1:B:95:GLU:O	1:B:99:LYS:HD3	1.89	0.72
1:C:30:MET:HG3	1:C:31:PHE:N	2.05	0.71
1:C:99:LYS:NZ	1:C:102:GLU:OE1	2.24	0.70
1:A:118:PHE:CZ	1:A:139:LEU:HD13	2.27	0.69
1:C:201:PRO:HB2	1:C:281:MET:SD	2.32	0.69
1:A:44:ARG:HH21	1:A:291:LYS:HG3	1.58	0.68
1:C:98:LEU:O	1:C:102:GLU:HG3	1.92	0.68
1:B:118:PHE:CZ	1:B:139:LEU:HD13	2.29	0.67
1:B:44:ARG:HD2	1:B:81:LEU:O	1.95	0.66
1:C:188:ASN:OD1	1:C:223:VAL:HB	1.96	0.65
1:C:32:ASP:HB3	1:C:35:GLU:HB2	1.78	0.64
1:C:145:GLY:HA2	1:C:152:VAL:HG22	1.78	0.64
1:C:285:LYS:NZ	1:D:247:GLU:OE1	2.33	0.62
1:A:203:GLY:O	1:A:206:PHE:HB2	2.00	0.61
1:D:203:GLY:O	1:D:206:PHE:HB2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:ASP:N	1:D:110:ASP:OD1	2.33	0.61
1:B:166:ASN:N	1:B:166:ASN:OD1	2.34	0.60
1:D:48:LEU:HD23	1:D:86:LYS:HB2	1.85	0.58
1:D:48:LEU:HD11	1:D:103:VAL:HG21	1.86	0.57
1:C:108:HIS:H	1:C:150:SER:CB	2.18	0.56
1:A:102:GLU:O	1:A:106:VAL:HG23	2.05	0.56
1:A:44:ARG:NH1	1:A:81:LEU:O	2.39	0.56
1:C:118:PHE:CE2	1:C:139:LEU:HD13	2.40	0.56
2:G:46:THR:HG23	2:G:48:LEU:CD1	2.36	0.56
1:C:44:ARG:HD2	1:C:81:LEU:O	2.07	0.55
1:B:75:THR:O	1:B:85:VAL:HG21	2.07	0.55
2:G:50:ARG:C	2:H:39:ARG:NH1	2.59	0.55
1:A:281:MET:SD	1:B:277:CYS:HB3	2.47	0.55
1:B:57:TRP:CZ2	2:G:50:ARG:C	2.80	0.54
1:B:263:PHE:O	1:B:263:PHE:CD1	2.61	0.54
1:C:37:TYR:CD2	1:C:155:PRO:HG3	2.43	0.53
1:A:73:ASN:O	1:A:76:ARG:HG2	2.10	0.52
1:A:239:TYR:HB3	1:A:243:LEU:HD22	1.91	0.52
1:D:201:PRO:HB2	1:D:281:MET:SD	2.49	0.52
1:A:118:PHE:HB3	1:A:127:ILE:CD1	2.40	0.52
1:A:118:PHE:HZ	1:A:139:LEU:HD13	1.71	0.52
2:H:42:CYS:SG	2:H:44:GLU:O	2.68	0.51
1:C:203:GLY:O	1:C:206:PHE:HB2	2.11	0.51
1:C:262:ASP:HB3	1:C:264:CYS:HB3	1.90	0.51
1:C:199:THR:HG22	1:C:210:TYR:CG	2.45	0.51
1:A:262:ASP:O	1:A:264:CYS:N	2.43	0.51
1:C:113:CYS:HB2	1:C:155:PRO:O	2.11	0.51
1:C:120:SER:O	1:C:162:ALA:HA	2.10	0.51
1:B:94:GLU:HG3	4:B:301:HOH:O	2.11	0.50
1:A:98:LEU:O	1:A:102:GLU:HG3	2.12	0.50
1:B:37:TYR:O	1:B:39:MET:HG2	2.12	0.50
1:A:270:ILE:HD12	1:A:270:ILE:N	2.26	0.49
1:C:118:PHE:CZ	1:C:139:LEU:HD13	2.48	0.49
1:B:93:ALA:HB3	2:H:45:TRP:CD1	2.47	0.49
1:B:201:PRO:HB2	1:B:281:MET:SD	2.52	0.49
1:D:220:ARG:HA	1:D:226:SER:HA	1.94	0.49
1:D:187:THR:HG23	1:D:189:ILE:HD11	1.95	0.49
1:B:73:ASN:O	1:B:77:ARG:HG2	2.13	0.48
1:B:43:ARG:NH2	4:B:329:HOH:O	2.32	0.48
1:C:48:LEU:HD11	1:C:103:VAL:HG21	1.95	0.48
1:C:265:LYS:HB3	1:C:265:LYS:HE2	1.65	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:GLY:HA2	1:B:152:VAL:HG22	1.96	0.48
1:B:203:GLY:O	1:B:206:PHE:HB2	2.14	0.48
1:A:118:PHE:HB3	1:A:127:ILE:HD11	1.96	0.48
1:C:108:HIS:HB2	1:C:150:SER:HB2	1.96	0.48
1:A:201:PRO:HB2	1:A:281:MET:SD	2.54	0.47
1:D:165:GLY:HA2	1:D:193:ASP:OD2	2.14	0.47
1:A:77:ARG:HD2	1:A:233:CYS:O	2.13	0.47
1:C:151:LEU:HA	1:C:154:LYS:HD2	1.96	0.47
1:A:100:ILE:HD13	1:A:139:LEU:HD22	1.96	0.47
1:D:94:GLU:HG2	2:H:40:LEU:HD13	1.96	0.47
1:A:44:ARG:HH21	1:A:291:LYS:CG	2.25	0.47
1:C:227:TRP:CD2	1:C:259:ARG:HD3	2.49	0.47
1:A:265:LYS:HE3	1:A:265:LYS:HA	1.96	0.46
2:E:48:LEU:HD22	2:F:41:HIS:HB2	1.97	0.46
1:B:219:HIS:HB2	1:B:227:TRP:CD2	2.50	0.46
1:A:65:ARG:O	1:A:220:ARG:HD2	2.15	0.46
1:B:164:ARG:HB2	1:B:196:SER:HB3	1.96	0.46
2:G:50:ARG:CA	2:H:39:ARG:HH12	2.28	0.46
1:C:34:ALA:HA	1:C:285:LYS:HE3	1.98	0.46
1:C:37:TYR:CG	1:C:155:PRO:HG3	2.51	0.46
1:B:211:SER:HA	1:B:228:TYR:CD1	2.51	0.46
1:D:118:PHE:HB3	1:D:127:ILE:CD1	2.46	0.46
1:A:141:GLY:O	1:A:147:LYS:HD2	2.17	0.45
1:B:266:ASP:O	1:B:268:SER:N	2.50	0.45
1:D:41:HIS:O	1:D:291:LYS:NZ	2.40	0.45
1:A:201:PRO:HA	1:A:208:MET:HG3	1.98	0.45
1:D:148:CYS:SG	1:D:151:LEU:HD12	2.56	0.45
1:C:226:SER:O	1:C:230:GLN:HG3	2.16	0.45
1:A:120:SER:O	1:A:162:ALA:HA	2.17	0.45
1:B:217:TYR:O	1:B:274:GLN:HB2	2.17	0.45
1:D:98:LEU:HG	2:H:40:LEU:HD11	1.98	0.45
1:A:139:LEU:HD23	1:A:139:LEU:HA	1.58	0.45
2:G:49:GLU:HG2	2:G:50:ARG:N	2.22	0.45
1:B:262:ASP:HA	1:B:270:ILE:HG23	2.00	0.44
1:C:41:HIS:HB2	1:C:112:ASP:OD1	2.17	0.44
1:C:264:CYS:O	1:C:264:CYS:SG	2.75	0.44
1:D:120:SER:O	1:D:162:ALA:HA	2.18	0.44
1:C:198:TYR:HA	4:C:453:HOH:O	2.18	0.44
1:B:266:ASP:N	1:B:267:PRO:HD3	2.33	0.44
1:C:97:LEU:HD22	2:F:47:ILE:HD11	1.99	0.44
2:H:49:GLU:O	2:H:50:ARG:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:VAL:HG12	1:A:107:SER:H	1.83	0.44
1:C:243:LEU:HG	4:C:416:HOH:O	2.17	0.44
1:D:58:HIS:CE1	2:H:48:LEU:HD22	2.53	0.44
1:A:44:ARG:HE	1:A:291:LYS:HD2	1.82	0.44
1:B:269:ALA:HA	1:B:272:LYS:HD2	1.99	0.44
1:A:255:LYS:O	1:A:258:GLN:HG2	2.18	0.43
2:G:39:ARG:HB2	2:H:48:LEU:O	2.18	0.43
1:B:35:GLU:HG3	4:B:335:HOH:O	2.18	0.43
1:C:163:ALA:HB3	3:C:301:PO4:O3	2.19	0.43
1:A:227:TRP:CD2	1:A:259:ARG:HD3	2.54	0.43
1:A:239:TYR:CB	1:A:243:LEU:HD22	2.49	0.43
1:B:97:LEU:HD21	1:B:134:ILE:HG21	2.01	0.43
1:B:48:LEU:HD21	1:B:103:VAL:HG21	2.00	0.43
1:B:123:GLU:O	1:B:123:GLU:HG3	2.18	0.43
1:C:106:VAL:HG12	1:C:107:SER:N	2.33	0.43
1:A:94:GLU:HB2	2:F:40:LEU:CD2	2.49	0.43
2:F:39:ARG:HG2	2:F:40:LEU:H	1.83	0.43
1:A:254:ARG:HB2	1:B:283:THR:HB	2.01	0.42
1:B:126:HIS:CD2	1:B:135:GLU:HG2	2.54	0.42
1:D:98:LEU:O	1:D:102:GLU:HG3	2.18	0.42
1:D:219:HIS:HB2	1:D:227:TRP:CD2	2.54	0.42
1:C:158:PHE:HB2	1:C:208:MET:SD	2.59	0.42
1:D:192:VAL:HG21	1:D:269:ALA:CB	2.49	0.42
2:G:47:ILE:C	2:G:48:LEU:HD12	2.39	0.42
1:D:77:ARG:O	1:D:81:LEU:HG	2.19	0.42
2:H:49:GLU:OE1	2:H:49:GLU:HA	2.18	0.42
1:A:93:ALA:HB2	1:A:132:ALA:HB3	2.02	0.42
1:D:95:GLU:O	1:D:99:LYS:HG2	2.19	0.42
1:A:120:SER:OG	1:A:121:HIS:N	2.52	0.42
1:B:273:LYS:HE2	1:B:273:LYS:HB3	1.80	0.41
1:A:199:THR:OG1	1:B:201:PRO:CD	2.68	0.41
1:B:30:MET:HG3	1:B:31:PHE:H	1.84	0.41
1:D:30:MET:HG3	1:D:31:PHE:N	2.36	0.41
1:A:248:LEU:O	1:A:251:LEU:HB2	2.21	0.41
1:C:220:ARG:HA	1:C:226:SER:HA	2.01	0.41
1:D:74:LEU:HD13	1:D:117:VAL:HG11	2.02	0.41
1:B:106:VAL:HG12	1:B:107:SER:N	2.35	0.41
1:B:266:ASP:C	1:B:268:SER:H	2.24	0.41
1:B:123:GLU:O	1:B:124:GLY:C	2.59	0.41
1:C:281:MET:HG2	1:D:277:CYS:HB3	2.03	0.41
1:B:41:HIS:O	1:B:291:LYS:NZ	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:THR:HG23	1:B:85:VAL:HG11	2.03	0.41
1:C:108:HIS:H	1:C:150:SER:HB2	1.85	0.41
1:C:117:VAL:HG22	1:C:159:ILE:HB	2.02	0.41
1:D:50:PHE:CE1	1:D:96:LEU:HG	2.56	0.41
1:B:101:HIS:O	1:B:105:THR:HG23	2.20	0.40
1:A:94:GLU:HB2	2:F:40:LEU:HD22	2.04	0.40
1:C:43:ARG:HD2	4:C:403:HOH:O	2.21	0.40
1:C:239:TYR:HB3	1:C:243:LEU:HD22	2.04	0.40
1:B:50:PHE:CE1	1:B:96:LEU:HG	2.57	0.40
1:C:31:PHE:CE2	1:D:254:ARG:NH2	2.90	0.40
1:D:267:PRO:HA	1:D:270:ILE:CD1	2.51	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	239/279 (86%)	224 (94%)	15 (6%)	0	100 100
1	B	239/279 (86%)	225 (94%)	12 (5%)	2 (1%)	19 28
1	C	239/279 (86%)	229 (96%)	10 (4%)	0	100 100
1	D	239/279 (86%)	231 (97%)	8 (3%)	0	100 100
2	E	10/18 (56%)	10 (100%)	0	0	100 100
2	F	9/18 (50%)	8 (89%)	1 (11%)	0	100 100
2	G	10/18 (56%)	9 (90%)	1 (10%)	0	100 100
2	H	10/18 (56%)	10 (100%)	0	0	100 100
All	All	995/1188 (84%)	946 (95%)	47 (5%)	2 (0%)	47 64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	124	GLY
1	B	267	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	210/245 (86%)	208 (99%)	2 (1%)	76 86
1	B	211/245 (86%)	206 (98%)	5 (2%)	49 67
1	C	210/245 (86%)	195 (93%)	15 (7%)	14 22
1	D	211/245 (86%)	205 (97%)	6 (3%)	43 61
2	E	11/17 (65%)	8 (73%)	3 (27%)	0 0
2	F	10/17 (59%)	9 (90%)	1 (10%)	7 10
2	G	12/17 (71%)	11 (92%)	1 (8%)	11 16
2	H	11/17 (65%)	11 (100%)	0	100 100
All	All	886/1048 (84%)	853 (96%)	33 (4%)	34 51

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	ASP
1	A	266	ASP
1	B	166	ASN
1	B	187	THR
1	B	189	ILE
1	B	220	ARG
1	B	268	SER
1	C	30	MET
1	C	36	LYS
1	C	42	ARG
1	C	44	ARG
1	C	53	GLU
1	C	95	GLU
1	C	99	LYS

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Mol	Chain	Res	Type
1	C	146	ASP
1	C	150	SER
1	C	166	ASN
1	C	193	ASP
1	C	255	LYS
1	C	264	CYS
1	C	266	ASP
1	C	268	SER
1	D	53	GLU
1	D	110	ASP
1	D	133	LYS
1	D	139	LEU
1	D	265	LYS
1	D	292	SER
2	E	39	ARG
2	E	48	LEU
2	E	49	GLU
2	F	39	ARG
2	G	40	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	224	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PO4	D	301	-	4,4,4	0.92	0	6,6,6	0.41	0
3	PO4	C	301	-	4,4,4	0.93	0	6,6,6	0.44	0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	301	PO4	1	0

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	242/279 (86%)	0.04	6 (2%) 57 53	22, 38, 78, 168	0
1	B	243/279 (87%)	0.09	12 (4%) 29 25	23, 37, 84, 151	0
1	C	243/279 (87%)	0.01	8 (3%) 46 43	22, 39, 86, 160	0
1	D	243/279 (87%)	-0.02	11 (4%) 33 30	21, 35, 83, 145	0
2	E	12/18 (66%)	0.41	2 (16%) 1 1	28, 51, 86, 94	0
2	F	11/18 (61%)	0.33	1 (9%) 9 7	28, 37, 67, 68	0
2	G	12/18 (66%)	1.04	3 (25%) 0 0	37, 51, 115, 124	0
2	H	12/18 (66%)	0.55	1 (8%) 11 9	33, 44, 87, 105	0
All	All	1018/1188 (85%)	0.05	44 (4%) 35 31	21, 38, 87, 168	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	263	PHE	10.9
1	B	264	CYS	8.8
1	D	264	CYS	7.9
1	C	263	PHE	7.7
2	G	50	ARG	6.5
1	A	264	CYS	6.4
1	B	267	PRO	6.3
1	D	263	PHE	6.2
1	B	262	ASP	5.4
1	B	261	VAL	5.4
1	B	263	PHE	5.3
1	A	262	ASP	5.3
1	C	261	VAL	5.2
1	D	265	LYS	5.1
1	C	264	CYS	5.0
2	E	50	ARG	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	269	ALA	4.5
1	A	269	ALA	4.4
1	C	262	ASP	4.3
1	B	265	LYS	4.2
1	B	260	ARG	4.0
1	A	30	MET	3.8
1	C	267	PRO	3.7
1	A	267	PRO	3.6
1	D	260	ARG	3.5
1	D	262	ASP	3.4
2	F	49	GLU	2.9
1	D	269	ALA	2.8
1	B	270	ILE	2.8
1	C	268	SER	2.7
2	G	48	LEU	2.7
1	D	261	VAL	2.6
2	G	49	GLU	2.6
1	B	268	SER	2.6
2	H	50	ARG	2.4
1	B	266	ASP	2.4
1	D	270	ILE	2.3
1	D	271	GLY	2.3
1	D	268	SER	2.2
1	C	187	THR	2.2
1	B	76	ARG	2.2
1	D	266	ASP	2.1
2	E	49	GLU	2.1
1	C	189	ILE	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 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
3	PO4	C	301	5/5	0.90	0.36	60,75,80,81	0
3	PO4	D	301	5/5	0.97	0.37	60,67,71,74	0

6.5 Other polymers (i)

There are no such residues in this entry.