Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2024 – 12:25 AM EDT

PDB ID	:	6C45
Title	:	Crystal structure of human inorganic pyrophosphatase in the P212121 space group
Authors	:	Niu, H.; Zhu, J.; Huang, X.; Du, Z.
Deposited on	:	2018-01-11
Resolution	:	2.39 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:

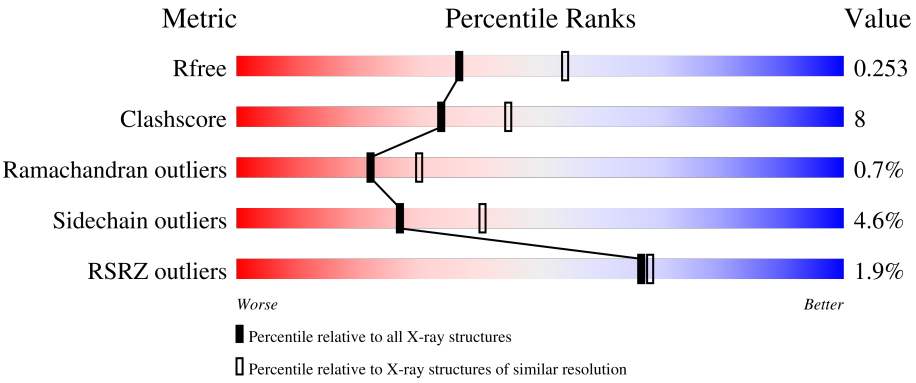
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.39 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	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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	289	81% 16%
1	B	289	79% 16%
1	C	289	81% 16%
1	D	289	4% 81% 14%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9557 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 Inorganic pyrophosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	0	0
			2278	1455	383	428	12			
1	B	282	Total	C	N	O	S	0	0	0
			2242	1434	375	421	12			
1	C	285	Total	C	N	O	S	0	0	0
			2269	1449	381	427	12			
1	D	282	Total	C	N	O	S	0	0	0
			2242	1433	374	423	12			

- Molecule 2 is water.

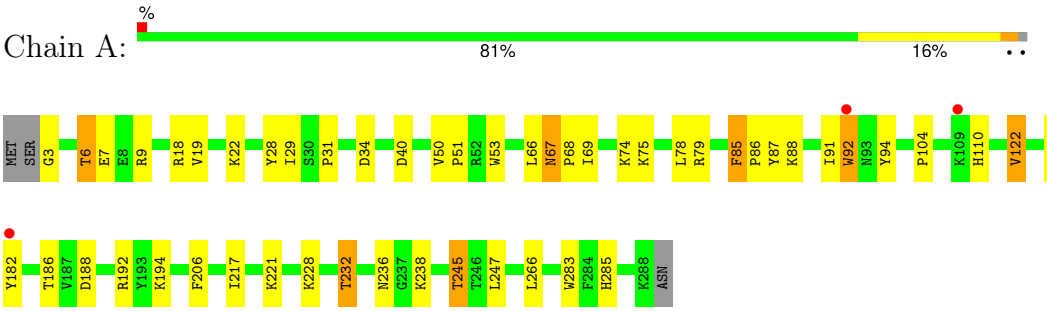
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	160	Total	O	0	0
			160	160		
2	B	179	Total	O	0	0
			179	179		
2	C	90	Total	O	0	0
			90	90		
2	D	97	Total	O	0	0
			97	97		

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.

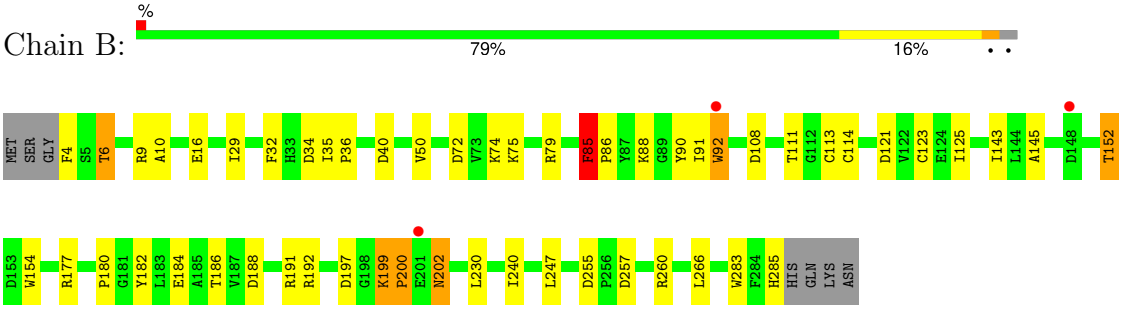
• Molecule 1: Inorganic pyrophosphatase

Chain A:



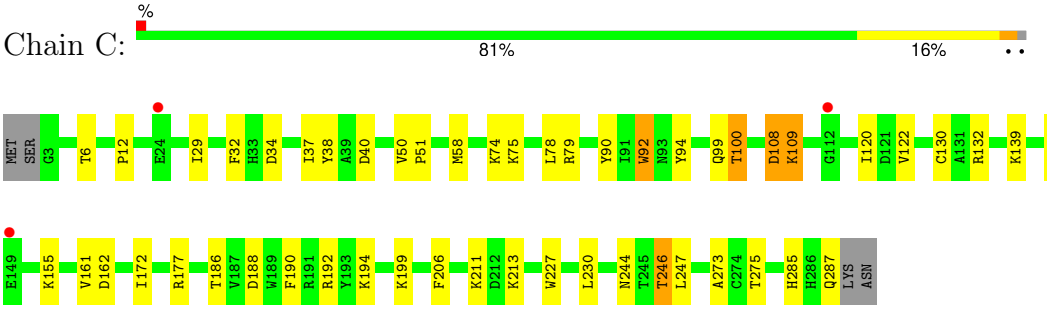
• Molecule 1: Inorganic pyrophosphatase

Chain B:



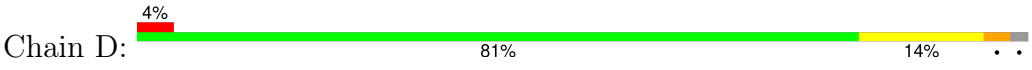
• Molecule 1: Inorganic pyrophosphatase

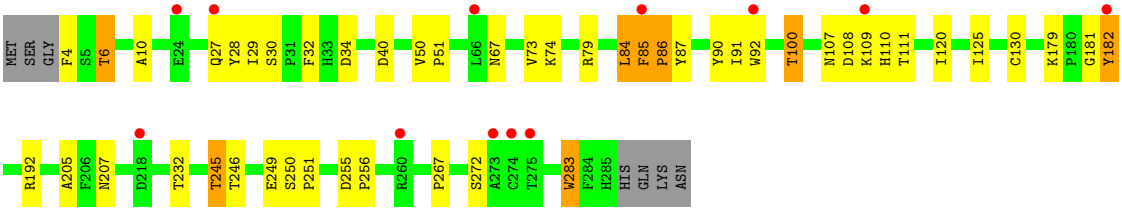
Chain C:



• Molecule 1: Inorganic pyrophosphatase

Chain D:




MET SER GLY F4 S5 T6 A10 E24 Q27 Y28 I29 S30 P31 F32 H33 D34 D40 V50 P51 L66 N67 V73 K74 R79 L84 F85 P86 Y87 Y90 I91 W92 T100 N107 D108 K109 H110 T111 I120 I125 C130 K179 P180 G181 Y182
R192 A205 P206 N207 D218 T232 T245 T246 E249 S250 P251 D255 P256 R260 P267 S272 A273 C274 T275 W283 P284 H285 HIS GLN LYS ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	50.25Å 136.94Å 216.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.28 – 2.39 84.90 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.8 (65.28-2.39) 99.8 (84.90-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.11 (at 2.40Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.193 , 0.251 0.198 , 0.253	Depositor DCC
R_{free} test set	2000 reflections (3.31%)	wwPDB-VP
Wilson B-factor (Å^2)	39.2	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 46.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9557	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.37% 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

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.45	0/2341	0.62	2/3177 (0.1%)
1	B	0.49	0/2305	0.66	1/3133 (0.0%)
1	C	0.40	0/2333	0.57	1/3170 (0.0%)
1	D	0.40	0/2304	0.56	0/3131
All	All	0.44	0/9283	0.60	4/12611 (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	A	0	2
1	B	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	85	PHE	C-N-CD	-8.16	102.65	120.60
1	B	85	PHE	C-N-CD	-7.54	104.02	120.60
1	A	122	VAL	CB-CA-C	-5.43	101.08	111.40
1	C	108	ASP	C-N-CA	5.06	134.35	121.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	66	LEU	Peptide
1	A	85	PHE	Peptide

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Mol	Chain	Res	Type	Group
1	B	85	PHE	Peptide
1	D	84	LEU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2278	0	2210	42	0
1	B	2242	0	2175	47	0
1	C	2269	0	2197	32	0
1	D	2242	0	2167	36	0
2	A	160	0	0	7	0
2	B	179	0	0	10	0
2	C	90	0	0	3	0
2	D	97	0	0	9	0
All	All	9557	0	8749	151	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 8.

All (151) 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:9:ARG:NH1	2:B:301:HOH:O	1.94	0.99
1:B:74:LYS:HG2	1:B:79:ARG:HD2	1.48	0.95
1:D:85:PHE:HB2	1:D:192:ARG:HH22	1.30	0.95
1:A:9:ARG:NH1	2:A:301:HOH:O	2.01	0.93
1:A:74:LYS:HG2	1:A:79:ARG:HD2	1.54	0.90
1:B:4:PHE:N	2:B:302:HOH:O	2.11	0.83
1:A:266:LEU:O	2:A:301:HOH:O	2.01	0.78
1:B:191:ARG:HG3	1:B:202:ASN:HB3	1.67	0.77
1:C:192:ARG:NH2	2:C:301:HOH:O	2.21	0.73
1:A:3:GLY:N	2:A:303:HOH:O	2.22	0.73
1:C:108:ASP:HA	1:C:109:LYS:HB2	1.73	0.71
1:D:249:GLU:O	2:D:301:HOH:O	2.09	0.71
1:C:177:ARG:NH2	2:C:303:HOH:O	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:THR:CG2	1:D:120:ILE:H	2.05	0.69
1:B:266:LEU:O	2:B:301:HOH:O	2.09	0.68
1:B:111:THR:HG22	1:B:113:CYS:H	1.57	0.68
1:A:192:ARG:NH2	2:A:304:HOH:O	2.24	0.68
1:B:192:ARG:NH2	2:B:306:HOH:O	2.27	0.67
1:B:257:ASP:OD1	1:B:260:ARG:NH2	2.24	0.67
1:A:285:HIS:HE1	1:B:182:TYR:HD1	1.41	0.67
1:B:92:TRP:CZ3	1:B:182:TYR:CZ	2.84	0.66
1:D:100:THR:HG21	1:D:120:ILE:HG22	1.77	0.66
1:D:125:ILE:HB	1:D:182:TYR:HE2	1.61	0.66
1:A:104:PRO:HG2	1:A:238:LYS:HD2	1.78	0.66
1:C:100:THR:CG2	1:C:120:ILE:H	2.09	0.66
1:C:100:THR:HG21	1:C:120:ILE:HG22	1.77	0.65
1:D:92:TRP:HZ3	1:D:182:TYR:CZ	2.15	0.65
1:A:7:GLU:HB2	1:A:22:LYS:HE2	1.78	0.65
1:D:245:THR:HG22	1:D:246:THR:HG23	1.80	0.64
1:A:285:HIS:CE1	1:B:182:TYR:HD1	2.15	0.64
1:D:50:VAL:HG11	1:D:90:TYR:CD2	2.33	0.64
1:B:202:ASN:OD1	1:B:202:ASN:N	2.31	0.63
1:B:91:ILE:HG13	1:B:92:TRP:CE2	2.34	0.62
1:D:91:ILE:HG13	1:D:92:TRP:CE2	2.34	0.62
1:C:139:LYS:HG3	1:C:161:VAL:HG12	1.82	0.61
1:D:4:PHE:N	2:D:305:HOH:O	2.32	0.61
1:A:50:VAL:HG22	1:A:94:TYR:HB3	1.81	0.60
1:D:10:ALA:HB2	1:D:267:PRO:HB2	1.83	0.60
1:B:184:GLU:OE1	2:B:303:HOH:O	2.16	0.60
1:A:92:TRP:NE1	2:A:302:HOH:O	2.14	0.60
1:B:111:THR:HG21	1:B:152:THR:HB	1.83	0.59
1:B:92:TRP:CZ3	1:B:182:TYR:CE2	2.90	0.59
1:B:92:TRP:CZ2	1:B:186:THR:OG1	2.55	0.59
1:A:91:ILE:HG13	1:A:92:TRP:CE2	2.38	0.59
1:A:91:ILE:HG13	1:A:92:TRP:CZ2	2.37	0.59
1:C:58:MET:HG2	1:C:132:ARG:HD3	1.85	0.58
1:B:50:VAL:HG11	1:B:90:TYR:CD2	2.38	0.58
1:D:92:TRP:HZ3	1:D:182:TYR:CE1	2.22	0.58
1:C:74:LYS:HG2	1:C:79:ARG:HD2	1.85	0.57
1:D:250:SER:HA	2:D:301:HOH:O	2.02	0.57
1:C:246:THR:HG22	1:C:247:LEU:HD23	1.86	0.57
1:A:217:ILE:HG22	1:A:221:LYS:HE2	1.86	0.57
1:D:125:ILE:HB	1:D:182:TYR:CE2	2.39	0.57
1:C:34:ASP:OD1	1:C:244:ASN:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:ASP:HB3	1:B:111:THR:HB	1.87	0.56
1:C:144:LEU:HB3	1:C:155:LYS:HB2	1.88	0.56
1:D:74:LYS:HG2	1:D:79:ARG:HD2	1.88	0.55
1:B:92:TRP:HE3	1:B:182:TYR:HH	1.54	0.55
1:B:180:PRO:HG3	2:B:395:HOH:O	2.06	0.55
1:A:285:HIS:HE1	1:B:182:TYR:CD1	2.22	0.54
1:C:100:THR:HG21	1:C:120:ILE:H	1.72	0.54
1:D:92:TRP:CZ3	1:D:182:TYR:CZ	2.95	0.53
1:A:92:TRP:CZ3	1:A:182:TYR:CZ	2.97	0.53
1:C:50:VAL:HG11	1:C:90:TYR:CD2	2.44	0.53
1:D:179:LYS:O	1:D:182:TYR:HB2	2.08	0.53
1:A:31:PRO:CG	1:A:67:ASN:HD22	2.23	0.52
1:B:85:PHE:HA	1:B:283:TRP:CZ3	2.44	0.52
1:D:85:PHE:CG	1:D:86:PRO:HD3	2.46	0.51
1:A:92:TRP:CZ2	1:A:186:THR:OG1	2.63	0.51
1:D:232:THR:HA	2:D:301:HOH:O	2.11	0.51
1:B:188:ASP:OD1	1:B:192:ARG:HD3	2.12	0.50
1:B:91:ILE:O	1:B:92:TRP:CE3	2.65	0.50
1:D:6:THR:HG21	2:D:358:HOH:O	2.11	0.50
1:B:121:ASP:OD1	2:B:304:HOH:O	2.19	0.50
1:A:28:TYR:O	1:A:245:THR:HG21	2.12	0.49
1:B:92:TRP:CE3	1:B:182:TYR:CZ	3.00	0.49
1:A:110:HIS:HB3	1:A:206:PHE:CZ	2.48	0.48
1:A:228:LYS:O	1:A:232:THR:HB	2.13	0.48
1:C:94:TYR:OH	1:C:155:LYS:HE3	2.13	0.48
1:A:285:HIS:CE1	1:B:182:TYR:CD1	2.99	0.48
1:A:67:ASN:HD21	1:A:68:PRO:CA	2.26	0.48
1:C:99:GLN:HG2	1:C:227:TRP:CZ2	2.49	0.48
1:A:67:ASN:OD1	1:A:68:PRO:N	2.47	0.47
1:B:6:THR:HB	2:B:390:HOH:O	2.13	0.47
1:C:58:MET:HG2	1:C:132:ARG:CD	2.43	0.47
1:A:188:ASP:OD1	1:A:192:ARG:HD3	2.15	0.47
1:C:108:ASP:CA	1:C:109:LYS:HB2	2.43	0.47
1:D:28:TYR:O	1:D:245:THR:HG21	2.15	0.47
1:D:251:PRO:HD3	2:D:301:HOH:O	2.15	0.47
1:A:92:TRP:CZ3	1:A:182:TYR:CE2	3.02	0.47
1:A:194:LYS:HG2	2:A:306:HOH:O	2.15	0.47
1:B:145:ALA:HB2	1:B:154:TRP:CZ3	2.50	0.47
1:B:230:LEU:HD21	1:B:240:ILE:HG21	1.97	0.47
1:A:91:ILE:O	1:A:92:TRP:CE3	2.68	0.46
1:A:92:TRP:HE3	1:A:182:TYR:HH	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:ASP:OD1	1:C:192:ARG:HD3	2.16	0.46
1:A:6:THR:HG22	2:A:394:HOH:O	2.13	0.46
1:C:29:ILE:HB	1:C:34:ASP:HB2	1.98	0.46
1:C:37:ILE:HG23	1:C:38:TYR:CD2	2.51	0.46
1:B:72:ASP:HB3	1:B:79:ARG:HD3	1.98	0.46
1:C:108:ASP:HA	1:C:109:LYS:CB	2.42	0.46
1:D:107:ASN:O	1:D:109:LYS:HG3	2.16	0.45
1:D:50:VAL:HG11	1:D:90:TYR:CE2	2.51	0.45
1:A:92:TRP:CE3	1:A:182:TYR:CZ	3.04	0.45
1:B:177:ARG:HD3	2:B:418:HOH:O	2.17	0.45
1:C:206:PHE:CD2	1:C:211:LYS:HE2	2.51	0.45
1:D:181:GLY:O	2:D:302:HOH:O	2.21	0.45
1:C:155:LYS:HE2	1:C:190:PHE:CE1	2.51	0.44
1:D:111:THR:HG22	1:D:205:ALA:HB2	1.99	0.44
1:B:9:ARG:HA	1:B:9:ARG:HD3	1.67	0.44
1:C:92:TRP:HZ3	1:C:186:THR:OG1	2.00	0.44
1:C:142:GLY:HA3	1:C:172:ILE:HD13	1.99	0.44
1:A:180:PRO:HD2	1:B:285:HIS:HB3	2.00	0.44
1:C:12:PRO:HD2	1:C:273:ALA:HA	1.98	0.44
1:C:92:TRP:CZ3	1:C:186:THR:HG23	2.53	0.43
1:C:194:LYS:HB3	1:C:199:LYS:HB2	1.99	0.43
1:D:109:LYS:HA	1:D:110:HIS:CD2	2.54	0.43
1:A:236:ASN:OD1	1:A:238:LYS:HG2	2.18	0.43
1:B:125:ILE:HG22	1:B:182:TYR:HE2	1.83	0.43
1:B:143:ILE:HD11	1:B:154:TRP:HB3	2.01	0.43
1:D:51:PRO:HB3	1:D:130:CYS:O	2.18	0.43
1:B:199:LYS:HB2	1:B:200:PRO:HD3	2.01	0.42
1:B:92:TRP:CD1	1:B:123:CYS:HB3	2.53	0.42
1:B:35:ILE:HA	1:B:36:PRO:HD3	1.92	0.42
1:A:50:VAL:HA	1:A:51:PRO:HD3	1.83	0.42
1:C:285:HIS:O	2:C:302:HOH:O	2.22	0.42
1:A:18:ARG:HD2	1:A:68:PRO:CG	2.49	0.42
1:D:85:PHE:O	2:D:303:HOH:O	2.21	0.42
1:A:67:ASN:HD21	1:A:68:PRO:N	2.18	0.42
1:B:191:ARG:CG	1:B:202:ASN:HB3	2.44	0.42
1:D:29:ILE:HB	1:D:34:ASP:HB2	2.02	0.41
1:A:87:TYR:O	1:A:283:TRP:HZ3	2.03	0.41
1:D:87:TYR:O	1:D:283:TRP:HZ3	2.03	0.41
1:B:91:ILE:HG13	1:B:92:TRP:CZ2	2.55	0.41
1:B:202:ASN:ND2	2:B:321:HOH:O	2.47	0.41
1:C:51:PRO:HB3	1:C:130:CYS:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:LYS:HE2	1:C:213:LYS:HB3	1.86	0.41
1:B:10:ALA:CB	1:B:16:GLU:HG2	2.50	0.41
1:D:108:ASP:OD2	1:D:111:THR:HG23	2.19	0.41
1:D:232:THR:HG22	2:D:301:HOH:O	2.21	0.41
1:A:29:ILE:HB	1:A:34:ASP:HB2	2.03	0.41
1:B:114:CYS:O	1:B:152:THR:HG22	2.21	0.41
1:B:29:ILE:HB	1:B:34:ASP:HB2	2.02	0.41
1:C:92:TRP:CH2	1:C:186:THR:HG23	2.56	0.41
1:D:30:SER:OG	1:D:67:ASN:OD1	2.27	0.40
1:D:108:ASP:CG	1:D:110:HIS:HB2	2.42	0.40
1:A:51:PRO:HB3	1:A:130:CYS:O	2.21	0.40
1:A:92:TRP:HZ2	1:A:186:THR:HA	1.86	0.40
1:A:19:VAL:HB	1:A:69:ILE:HB	2.03	0.40
1:A:53:TRP:CD2	1:B:88:LYS:HG3	2.57	0.40
1:D:27:GLN:OE1	1:D:256:PRO:HG3	2.20	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	282/289 (98%)	278 (99%)	3 (1%)	1 (0%)	34	46
1	B	280/289 (97%)	270 (96%)	7 (2%)	3 (1%)	14	18
1	C	283/289 (98%)	272 (96%)	10 (4%)	1 (0%)	34	46
1	D	278/289 (96%)	265 (95%)	10 (4%)	3 (1%)	14	18
All	All	1123/1156 (97%)	1085 (97%)	30 (3%)	8 (1%)	22	30

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	PRO
1	B	86	PRO
1	B	199	LYS
1	B	200	PRO
1	C	109	LYS
1	D	85	PHE
1	D	86	PRO
1	D	272	SER

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	247/250 (99%)	236 (96%)	11 (4%)	27	41
1	B	243/250 (97%)	233 (96%)	10 (4%)	30	45
1	C	246/250 (98%)	233 (95%)	13 (5%)	22	34
1	D	243/250 (97%)	232 (96%)	11 (4%)	27	41
All	All	979/1000 (98%)	934 (95%)	45 (5%)	27	40

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	THR
1	A	40	ASP
1	A	67	ASN
1	A	75	LYS
1	A	78	LEU
1	A	88	LYS
1	A	92	TRP
1	A	122	VAL
1	A	232	THR
1	A	245	THR
1	A	247	LEU
1	B	6	THR
1	B	32	PHE
1	B	40	ASP

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Mol	Chain	Res	Type
1	B	75	LYS
1	B	92	TRP
1	B	152	THR
1	B	197	ASP
1	B	202	ASN
1	B	247	LEU
1	B	255	ASP
1	C	6	THR
1	C	32	PHE
1	C	40	ASP
1	C	75	LYS
1	C	78	LEU
1	C	92	TRP
1	C	100	THR
1	C	122	VAL
1	C	162	ASP
1	C	230	LEU
1	C	246	THR
1	C	275	THR
1	C	287	GLN
1	D	6	THR
1	D	32	PHE
1	D	40	ASP
1	D	73	VAL
1	D	84	LEU
1	D	100	THR
1	D	182	TYR
1	D	207	ASN
1	D	245	THR
1	D	255	ASP
1	D	283	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	285	HIS
1	D	27	GLN

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

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	67:ASN	C	68:PRO	N	6.00
1	D	109:LYS	C	110:HIS	N	5.08

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	286/289 (98%)	0.05	3 (1%)	82	83	7, 19, 39, 63	0
1	B	282/289 (97%)	0.09	3 (1%)	80	81	4, 13, 42, 67	0
1	C	285/289 (98%)	0.22	3 (1%)	80	81	15, 29, 52, 67	0
1	D	282/289 (97%)	0.40	12 (4%)	35	38	14, 29, 55, 70	0
All	All	1135/1156 (98%)	0.19	21 (1%)	66	68	4, 24, 49, 70	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	275	THR	6.4
1	D	109	LYS	4.9
1	B	92	TRP	4.8
1	B	201	GLU	4.6
1	D	85	PHE	4.4
1	D	182	TYR	4.0
1	A	92	TRP	3.6
1	D	92	TRP	3.2
1	C	112	GLY	2.8
1	D	273	ALA	2.8
1	A	109	LYS	2.8
1	D	274	CYS	2.7
1	D	27	GLN	2.6
1	B	148	ASP	2.5
1	D	24	GLU	2.4
1	A	182	TYR	2.3
1	D	66	LEU	2.2
1	D	218	ASP	2.2
1	D	260	ARG	2.1
1	C	149	GLU	2.1
1	C	24	GLU	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.