Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2021 – 10:40 AM EDT

PDB ID	:	1AUW
Title	:	H91N DELTA 2 CRYSTALLIN FROM DUCK
Authors	:	Abu-Abed, M.; Vallee, F.; Howell, P.L.
Deposited on	:	1997-09-03
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 ⓘ symbol.

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

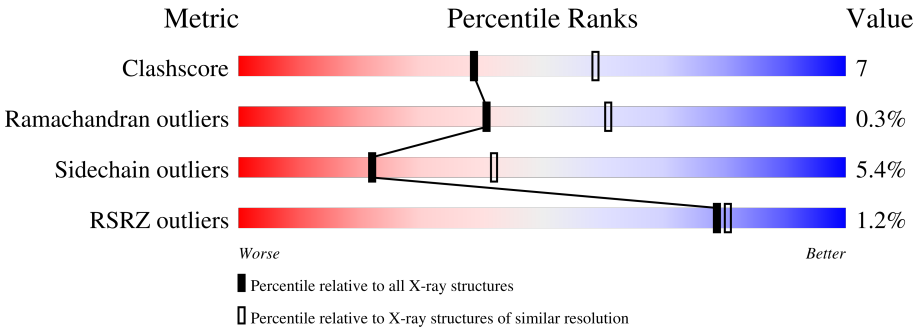
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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	468	76% 19%
1	B	468	76% 17%
1	C	468	73% 21%
1	D	468	77% 17%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 14215 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 DELTA 2 CRYSTALLIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	447	Total	C	N	O	S	0	0	0
			3468	2195	587	674	12			
1	B	447	Total	C	N	O	S	0	0	0
			3468	2195	587	674	12			
1	C	447	Total	C	N	O	S	0	0	0
			3468	2195	587	674	12			
1	D	447	Total	C	N	O	S	0	0	0
			3468	2195	587	674	12			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	89	ASN	HIS	engineered mutation	UNP P24058
A	273	ASP	LEU	conflict	UNP P24058
A	441	GLY	ALA	conflict	UNP P24058
B	89	ASN	HIS	engineered mutation	UNP P24058
B	273	ASP	LEU	conflict	UNP P24058
B	441	GLY	ALA	conflict	UNP P24058
C	89	ASN	HIS	engineered mutation	UNP P24058
C	273	ASP	LEU	conflict	UNP P24058
C	441	GLY	ALA	conflict	UNP P24058
D	89	ASN	HIS	engineered mutation	UNP P24058
D	273	ASP	LEU	conflict	UNP P24058
D	441	GLY	ALA	conflict	UNP P24058

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	106	Total	O	0	0
			106	106		
2	B	91	Total	O	0	0
			91	91		

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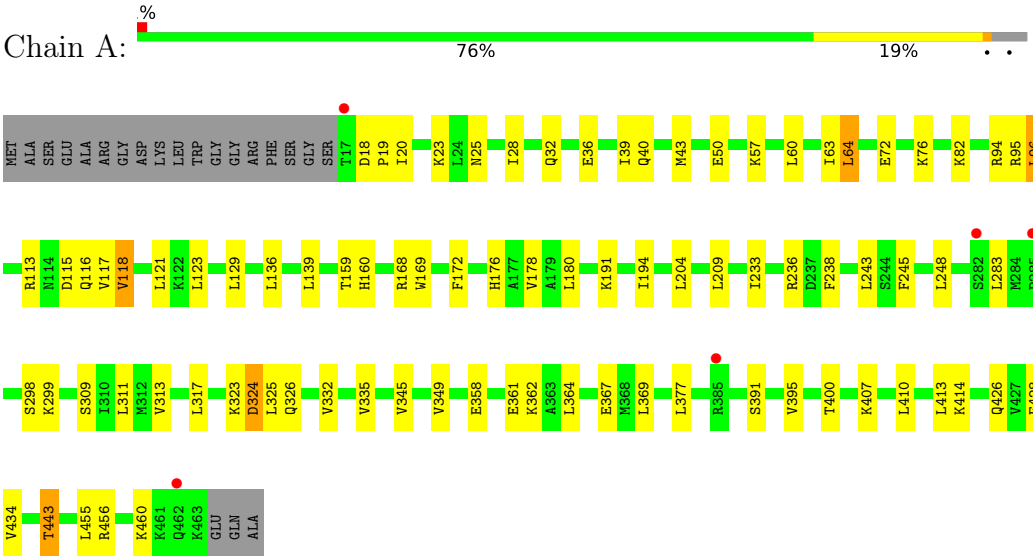
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	68	Total O 68 68	0	0
2	D	78	Total O 78 78	0	0

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.

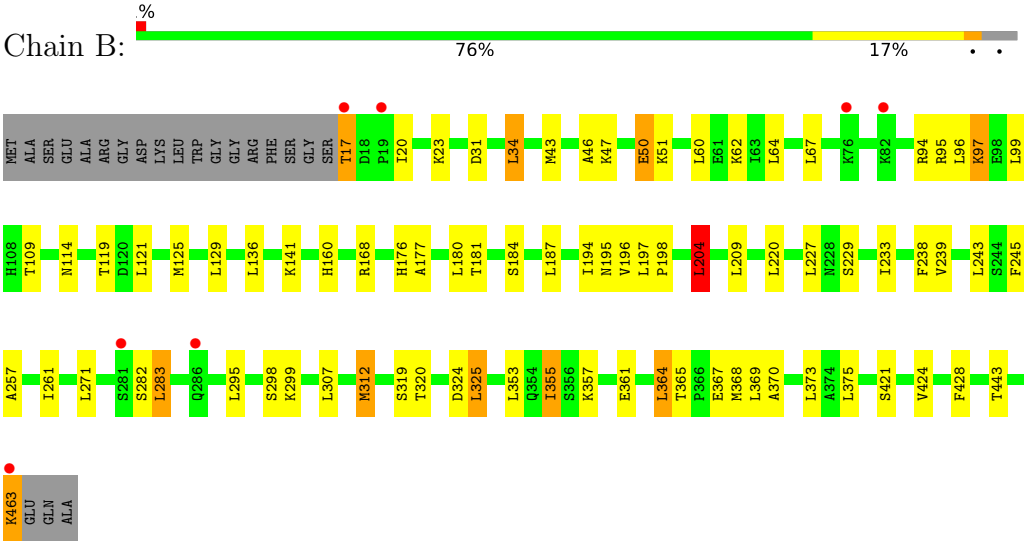
• Molecule 1: DELTA 2 CRYSTALLIN

Chain A:



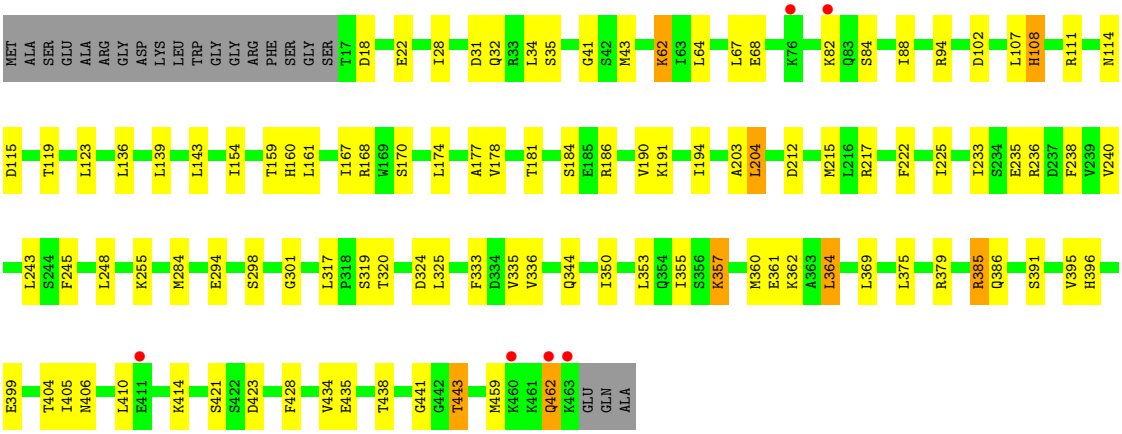
• Molecule 1: DELTA 2 CRYSTALLIN

Chain B:



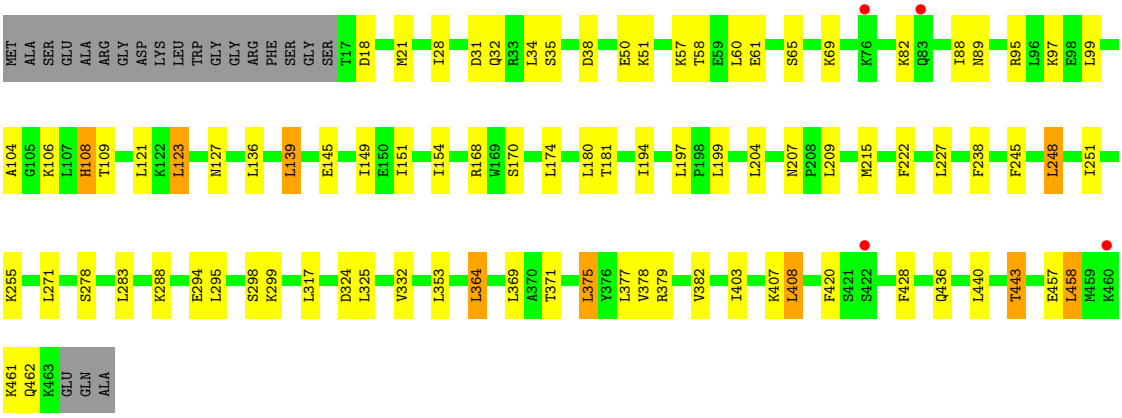
• Molecule 1: DELTA 2 CRYSTALLIN

Chain C:



• Molecule 1: DELTA 2 CRYSTALLIN

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	94.10Å 100.20Å 109.10Å 90.00° 102.10° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50 24.34 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.0 (8.00-2.50) 89.7 (24.34-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	6.04 (at 2.50Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.161 , 0.235 0.164 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	30.4	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 85.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14215	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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	0.36	0/3512	0.57	0/4736
1	B	0.36	0/3512	0.58	1/4736 (0.0%)
1	C	0.35	0/3512	0.57	0/4736
1	D	0.35	0/3512	0.57	0/4736
All	All	0.36	0/14048	0.57	1/18944 (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	B	204	LEU	CA-CB-CG	6.34	129.88	115.30

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	3468	0	3585	48	0
1	B	3468	0	3585	57	0
1	C	3468	0	3585	70	0
1	D	3468	0	3585	55	0
2	A	106	0	0	2	0
2	B	91	0	0	1	0
2	C	68	0	0	3	0
2	D	78	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	14215	0	14340	211	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (211) 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:129:LEU:HD22	1:B:187:LEU:HD11	1.55	0.89
1:C:82:LYS:HE3	1:C:84:SER:HB2	1.55	0.88
1:A:109:THR:HG22	1:A:209:LEU:HD11	1.60	0.83
1:B:168:ARG:HG3	1:B:443:THR:HG22	1.72	0.71
1:C:143:LEU:HD12	1:C:350:ILE:HG21	1.72	0.71
1:C:355:ILE:HB	1:C:360:MET:CE	2.22	0.70
1:C:62:LYS:HE2	1:C:62:LYS:HA	1.74	0.70
1:B:312:MET:HG2	1:C:301:GLY:HA2	1.74	0.69
1:A:358:GLU:O	1:A:362:LYS:HG2	1.94	0.68
1:D:97:LYS:HG2	1:D:104:ALA:HB3	1.74	0.68
1:C:115:ASP:HB3	1:C:233:ILE:HD11	1.75	0.67
1:C:82:LYS:CE	1:C:84:SER:HB2	2.25	0.67
1:B:50:GLU:HG2	1:B:60:LEU:HD22	1.78	0.66
1:D:65:SER:O	1:D:69:LYS:HD3	1.95	0.66
1:A:369:LEU:HD13	1:A:428:PHE:HA	1.76	0.65
1:B:20:ILE:O	1:B:23:LYS:HG2	1.97	0.64
1:B:109:THR:HG22	1:B:209:LEU:HD11	1.80	0.63
1:A:456:ARG:O	1:A:460:LYS:HG2	1.99	0.63
1:B:357:LYS:O	1:B:361:GLU:HG2	1.99	0.62
1:A:113:ARG:HH11	1:A:116:GLN:HE22	1.47	0.62
1:C:82:LYS:HE2	1:C:94:ARG:HD3	1.82	0.61
1:C:217:ARG:HH11	1:C:217:ARG:HG2	1.66	0.61
1:D:197:LEU:HD11	1:D:199:LEU:HB3	1.83	0.61
1:C:385:ARG:H	1:C:385:ARG:HD3	1.65	0.60
1:D:51:LYS:HD3	1:D:215:MET:SD	2.40	0.60
1:A:28:ILE:O	1:A:32:GLN:HG3	2.02	0.60
1:A:410:LEU:O	1:A:414:LYS:HG2	2.02	0.59
1:B:324:ASP:HA	1:C:298:SER:HB3	1.84	0.59
1:D:121:LEU:HD11	1:D:332:VAL:HG21	1.85	0.59
1:C:355:ILE:HB	1:C:360:MET:HE1	1.84	0.59
1:C:355:ILE:HB	1:C:360:MET:HE3	1.84	0.59
1:D:271:LEU:HD13	1:D:353:LEU:HD11	1.85	0.58
1:D:109:THR:HG22	1:D:209:LEU:HD11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:LEU:HB3	1:B:355:ILE:HD12	1.87	0.57
1:B:449:THR:O	1:B:453:GLU:HG2	2.05	0.57
1:B:95:ARG:NH2	1:B:99:LEU:HD21	2.20	0.56
1:B:176:HIS:HD2	2:B:534:HOH:O	1.87	0.56
1:C:108:HIS:HD2	1:C:111:ARG:HH21	1.54	0.56
1:D:375:LEU:HB3	1:D:379:ARG:HH12	1.71	0.56
1:D:375:LEU:HB3	1:D:379:ARG:NH1	2.21	0.56
1:D:457:GLU:O	1:D:461:LYS:HD3	2.05	0.56
1:D:50:GLU:HB2	1:D:60:LEU:HD22	1.90	0.54
1:A:367:GLU:HG2	1:C:284:MET:HG2	1.88	0.54
1:C:369:LEU:HD13	1:C:428:PHE:HA	1.89	0.54
1:C:186:ARG:O	1:C:190:VAL:HG13	2.08	0.54
1:B:17:THR:HG21	1:C:344:GLN:HB3	1.89	0.53
1:B:295:LEU:O	1:B:299:LYS:HG2	2.08	0.53
1:A:317:LEU:O	1:B:255:LYS:HG3	2.08	0.53
1:A:243:LEU:HD22	1:A:335:VAL:HG21	1.90	0.53
1:A:168:ARG:HG3	1:A:434:VAL:HG11	1.91	0.53
1:A:295:LEU:O	1:A:299:LYS:HG2	2.09	0.52
1:B:194:ILE:HG12	1:B:238:PHE:HB2	1.91	0.52
1:A:113:ARG:NH1	1:A:116:GLN:HE22	2.08	0.52
1:B:298:SER:HB3	1:C:324:ASP:HA	1.91	0.52
1:C:385:ARG:HH12	1:D:106:LYS:HG2	1.75	0.52
1:A:294:GLU:OE1	1:C:160:HIS:HD2	1.93	0.52
1:D:170:SER:O	1:D:174:LEU:HG	2.09	0.52
1:D:154:ILE:HG22	1:D:364:LEU:HD21	1.92	0.52
1:C:410:LEU:HD11	1:C:414:LYS:NZ	2.26	0.51
1:C:375:LEU:HB3	1:C:379:ARG:NH1	2.26	0.51
1:C:174:LEU:O	1:C:178:VAL:HG23	2.10	0.51
1:C:18:ASP:O	1:C:22:GLU:HG3	2.11	0.50
1:B:463:LYS:HD3	1:B:463:LYS:N	2.25	0.50
1:D:207:ASN:ND2	1:D:209:LEU:H	2.10	0.50
1:D:461:LYS:HD2	1:D:461:LYS:N	2.26	0.50
1:B:121:LEU:HD13	1:B:125:MET:CE	2.42	0.49
1:C:123:LEU:HD13	1:C:222:PHE:CZ	2.47	0.49
1:D:28:ILE:O	1:D:32:GLN:HG3	2.12	0.49
1:A:115:ASP:HB3	1:A:233:ILE:HD11	1.93	0.49
1:A:168:ARG:H	1:A:443:THR:CG2	2.24	0.49
1:A:194:ILE:HG12	1:A:238:PHE:HB2	1.94	0.49
1:A:298:SER:HB3	1:D:324:ASP:HA	1.94	0.49
1:D:88:ILE:HG23	1:D:89:ASN:N	2.28	0.49
1:A:168:ARG:H	1:A:443:THR:HG21	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:ARG:H	1:C:443:THR:HG21	1.76	0.49
1:A:169:TRP:O	1:A:172:PHE:HB3	2.13	0.49
1:A:159:THR:HG22	1:A:160:HIS:ND1	2.27	0.49
1:C:361:GLU:HG3	1:C:362:LYS:N	2.28	0.49
1:C:385:ARG:HG2	1:C:386:GLN:OE1	2.13	0.49
1:A:430:PHE:O	1:A:433:SER:HB3	2.12	0.49
1:C:395:VAL:HG12	1:C:405:ILE:HG21	1.94	0.49
1:B:62:LYS:HE2	1:B:100:ILE:HG23	1.94	0.48
1:B:187:LEU:HD13	1:B:245:PHE:CE2	2.47	0.48
1:B:368:MET:HB2	1:B:368:MET:HE2	1.70	0.48
1:C:43:MET:HG2	1:C:67:LEU:HD13	1.95	0.48
1:D:32:GLN:HA	1:D:88:ILE:HD13	1.96	0.48
1:B:312:MET:HG2	1:C:301:GLY:CA	2.44	0.48
1:A:178:VAL:HG12	1:A:455:LEU:HD21	1.94	0.48
1:A:361:GLU:HA	1:A:364:LEU:HD23	1.96	0.48
1:D:403:ILE:HD11	1:D:408:LEU:HD12	1.96	0.48
1:A:129:LEU:HB3	1:A:191:LYS:HE2	1.96	0.48
1:B:229:SER:O	1:B:233:ILE:HG12	2.14	0.48
1:D:379:ARG:HH22	1:D:436:GLN:NE2	2.12	0.48
1:B:168:ARG:H	1:B:443:THR:CG2	2.25	0.48
1:C:435:GLU:O	1:C:438:THR:HG23	2.13	0.48
1:D:57:LYS:O	1:D:61:GLU:HG3	2.14	0.47
1:B:365:THR:HG22	1:B:367:GLU:H	1.78	0.47
1:B:168:ARG:H	1:B:443:THR:HG21	1.79	0.47
1:D:123:LEU:HD13	1:D:222:PHE:CZ	2.49	0.47
1:D:123:LEU:HD13	1:D:222:PHE:CE2	2.49	0.47
1:B:160:HIS:HA	1:D:294:GLU:OE2	2.15	0.47
1:B:421:SER:O	1:B:424:VAL:HG12	2.14	0.47
1:B:369:LEU:HD13	1:B:428:PHE:HA	1.96	0.47
1:C:255:LYS:HD2	2:D:515:HOH:O	2.14	0.47
1:A:283:LEU:HD22	1:C:391:SER:HB2	1.97	0.47
1:A:358:GLU:O	1:A:361:GLU:HG2	2.14	0.47
1:D:369:LEU:HD13	1:D:428:PHE:HA	1.95	0.47
1:D:295:LEU:O	1:D:299:LYS:HG2	2.15	0.47
1:C:217:ARG:HG2	1:C:217:ARG:NH1	2.29	0.46
1:C:375:LEU:HB3	1:C:379:ARG:HH12	1.79	0.46
1:C:396:HIS:O	1:C:399:GLU:HB3	2.14	0.46
1:B:184:SER:HB3	1:B:462:GLN:NE2	2.29	0.46
1:A:324:ASP:HA	1:D:298:SER:HB3	1.97	0.46
1:C:170:SER:O	1:C:174:LEU:HG	2.15	0.46
1:C:391:SER:O	1:C:395:VAL:HG13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:194:ILE:HG12	1:D:238:PHE:HB2	1.97	0.46
1:A:72:GLU:HG2	1:A:76:LYS:HE2	1.98	0.46
1:B:353:LEU:CD1	1:B:355:ILE:HD13	2.46	0.46
1:C:119:THR:O	1:C:123:LEU:HB2	2.15	0.46
1:B:364:LEU:HA	1:B:368:MET:HE1	1.98	0.45
1:B:50:GLU:HG3	1:B:51:LYS:N	2.31	0.45
1:C:333:PHE:O	1:C:336:VAL:HG22	2.16	0.45
1:C:194:ILE:HG12	1:C:238:PHE:HB2	1.98	0.45
1:D:377:LEU:HD11	1:D:420:PHE:CZ	2.52	0.45
1:B:257:ALA:O	1:B:261:ILE:HG13	2.17	0.45
1:C:154:ILE:HD13	1:C:434:VAL:HG21	1.98	0.45
1:A:391:SER:O	1:A:395:VAL:HG23	2.17	0.45
1:A:39:ILE:O	1:A:43:MET:HG3	2.16	0.45
1:C:114:ASN:HB3	1:C:233:ILE:HG23	1.99	0.45
1:B:177:ALA:O	1:B:181:THR:HG23	2.16	0.45
1:D:82:LYS:HB2	1:D:82:LYS:NZ	2.32	0.45
1:D:18:ASP:HB3	1:D:21:MET:HB2	1.98	0.44
1:C:212:ASP:OD2	1:C:215:MET:HB2	2.17	0.44
1:B:31:ASP:O	1:B:34:LEU:HB2	2.18	0.44
1:C:28:ILE:O	1:C:32:GLN:HG3	2.18	0.44
1:B:100:ILE:HG22	1:B:103:ILE:HB	1.99	0.44
1:C:161:LEU:HD23	1:C:161:LEU:HA	1.86	0.44
1:C:243:LEU:HD22	1:C:335:VAL:HG21	2.00	0.44
1:B:196:VAL:O	1:B:198:PRO:HD3	2.18	0.44
1:C:459:MET:O	1:C:462:GLN:HB3	2.17	0.44
1:D:168:ARG:H	1:D:443:THR:CG2	2.31	0.44
1:A:243:LEU:CD2	1:A:335:VAL:HG21	2.48	0.44
1:B:114:ASN:HB3	1:B:233:ILE:HG23	1.99	0.44
1:B:319:SER:HA	1:B:320:THR:HA	1.76	0.44
1:C:28:ILE:HA	1:C:31:ASP:OD1	2.18	0.44
1:C:203:ALA:O	1:C:204:LEU:HB3	2.17	0.44
1:B:43:MET:O	1:B:47:LYS:HG3	2.17	0.43
1:D:378:VAL:HA	1:D:382:VAL:O	2.18	0.43
1:B:43:MET:HG2	1:B:67:LEU:HD13	1.98	0.43
1:D:145:GLU:O	1:D:149:ILE:HG12	2.18	0.43
1:B:141:LYS:O	1:B:141:LYS:HD3	2.19	0.43
1:C:108:HIS:CD2	1:C:111:ARG:HE	2.36	0.43
1:A:50:GLU:HG3	1:A:60:LEU:HD22	1.99	0.43
1:C:357:LYS:HZ2	1:C:357:LYS:HB2	1.82	0.43
1:D:139:LEU:HD13	1:D:180:LEU:HD13	2.00	0.43
1:C:177:ALA:O	1:C:181:THR:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:HIS:ND1	1:D:108:HIS:N	2.67	0.43
1:A:36:GLU:O	1:A:40:GLN:HG2	2.19	0.43
1:C:191:LYS:HG2	2:C:492:HOH:O	2.18	0.43
1:C:240:VAL:HG11	1:D:248:LEU:HG	2.00	0.43
1:B:443:THR:HG22	1:B:443:THR:O	2.19	0.43
1:C:168:ARG:H	1:C:443:THR:CG2	2.32	0.43
1:A:118:VAL:HG13	1:A:236:ARG:NH2	2.33	0.42
1:D:127:ASN:N	1:D:127:ASN:HD22	2.15	0.42
1:B:46:ALA:HB2	1:B:107:LEU:HD21	2.00	0.42
1:C:255:LYS:HG3	1:D:317:LEU:O	2.20	0.42
1:A:20:ILE:O	1:A:23:LYS:HG2	2.19	0.42
1:A:311:LEU:HD23	1:A:311:LEU:HA	1.86	0.42
1:D:168:ARG:H	1:D:443:THR:HG21	1.83	0.42
1:B:125:MET:HE1	1:B:239:VAL:HG22	2.00	0.42
1:C:64:LEU:O	1:C:68:GLU:HG3	2.19	0.42
1:D:251:ILE:HD13	1:D:251:ILE:HA	1.90	0.42
1:A:113:ARG:O	1:A:117:VAL:HG22	2.20	0.42
1:A:345:VAL:O	1:A:349:VAL:HG23	2.20	0.42
1:A:64:LEU:HD12	1:A:64:LEU:HA	1.88	0.42
1:B:283:LEU:HD23	1:D:371:THR:HG22	2.02	0.42
1:D:28:ILE:HA	1:D:31:ASP:OD1	2.20	0.42
1:D:151:ILE:HA	1:D:170:SER:OG	2.20	0.41
1:C:319:SER:HA	1:C:320:THR:HA	1.81	0.41
1:C:404:THR:HB	1:C:406:ASN:OD1	2.20	0.41
1:A:82:LYS:HD3	1:A:94:ARG:CZ	2.51	0.41
1:A:57:LYS:HD2	2:A:498:HOH:O	2.19	0.41
1:B:197:LEU:HD11	1:B:220:LEU:HD12	2.03	0.41
1:B:365:THR:H	1:B:368:MET:HE1	1.85	0.41
1:C:357:LYS:NZ	1:C:357:LYS:H	2.18	0.41
1:D:95:ARG:O	1:D:99:LEU:HG	2.20	0.41
1:D:278:SER:OG	1:D:288:LYS:HD2	2.21	0.41
1:B:325:LEU:HD12	1:B:325:LEU:HA	1.90	0.41
1:C:361:GLU:HA	1:C:364:LEU:CD2	2.51	0.41
1:A:176:HIS:HD2	2:A:561:HOH:O	2.03	0.41
1:B:62:LYS:HE2	1:B:62:LYS:HB3	1.93	0.41
1:B:94:ARG:O	1:B:97:LYS:HG3	2.20	0.41
1:B:353:LEU:HD12	1:B:353:LEU:C	2.41	0.41
1:C:35:SER:HB3	1:C:88:ILE:HD11	2.02	0.41
1:D:375:LEU:O	1:D:379:ARG:HG3	2.21	0.41
1:A:160:HIS:HD2	1:C:294:GLU:OE1	2.04	0.41
1:C:41:GLY:HA3	2:C:522:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:512:HOH:O	1:D:255:LYS:HB2	2.21	0.41
1:D:458:LEU:HA	1:D:458:LEU:HD12	1.86	0.41
1:A:309:SER:O	1:A:313:VAL:HG23	2.20	0.40
1:A:323:LYS:O	1:A:326:GLN:HG2	2.21	0.40
1:B:187:LEU:HD13	1:B:245:PHE:CZ	2.56	0.40
1:D:35:SER:O	1:D:38:ASP:HB3	2.21	0.40
1:B:370:ALA:O	1:B:373:LEU:HB3	2.22	0.40
1:C:421:SER:HB3	1:C:423:ASP:OD1	2.21	0.40
1:C:441:GLY:HA2	1:D:227:LEU:O	2.22	0.40
1:A:18:ASP:N	1:A:19:PRO:HD2	2.35	0.40
1:C:317:LEU:O	1:D:255:LYS:HG3	2.22	0.40
1:A:63:ILE:HG23	1:A:96:LEU:HD11	2.03	0.40
1:B:119:THR:OG1	1:B:198:PRO:HG2	2.22	0.40
1:D:461:LYS:O	1:D:462:GLN:HB2	2.22	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	445/468 (95%)	437 (98%)	7 (2%)	1 (0%)	47	68
1	B	445/468 (95%)	433 (97%)	11 (2%)	1 (0%)	47	68
1	C	445/468 (95%)	434 (98%)	10 (2%)	1 (0%)	47	68
1	D	445/468 (95%)	430 (97%)	13 (3%)	2 (0%)	34	54
All	All	1780/1872 (95%)	1734 (97%)	41 (2%)	5 (0%)	41	61

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	204	LEU

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Mol	Chain	Res	Type
1	C	204	LEU
1	D	440	LEU
1	B	204	LEU
1	D	204	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	390/405 (96%)	367 (94%)	23 (6%)	19	37
1	B	390/405 (96%)	368 (94%)	22 (6%)	21	40
1	C	390/405 (96%)	368 (94%)	22 (6%)	21	40
1	D	390/405 (96%)	373 (96%)	17 (4%)	28	52
All	All	1560/1620 (96%)	1476 (95%)	84 (5%)	22	42

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	64	LEU
1	A	95	ARG
1	A	96	LEU
1	A	99	LEU
1	A	118	VAL
1	A	121	LEU
1	A	123	LEU
1	A	136	LEU
1	A	139	LEU
1	A	180	LEU
1	A	245	PHE
1	A	248	LEU
1	A	286	GLN
1	A	324	ASP
1	A	325	LEU
1	A	332	VAL

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Mol	Chain	Res	Type
1	A	377	LEU
1	A	400	THR
1	A	407	LYS
1	A	413	LEU
1	A	426	GLN
1	A	443	THR
1	B	17	THR
1	B	34	LEU
1	B	50	GLU
1	B	64	LEU
1	B	96	LEU
1	B	97	LYS
1	B	136	LEU
1	B	180	LEU
1	B	195	ASN
1	B	204	LEU
1	B	227	LEU
1	B	243	LEU
1	B	248	LEU
1	B	282	SER
1	B	283	LEU
1	B	307	LEU
1	B	312	MET
1	B	325	LEU
1	B	355	ILE
1	B	364	LEU
1	B	375	LEU
1	B	463	LYS
1	C	34	LEU
1	C	62	LYS
1	C	102	ASP
1	C	107	LEU
1	C	108	HIS
1	C	136	LEU
1	C	139	LEU
1	C	159	THR
1	C	167	ILE
1	C	184	SER
1	C	225	ILE
1	C	235	GLU
1	C	236	ARG
1	C	245	PHE

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Mol	Chain	Res	Type
1	C	248	LEU
1	C	325	LEU
1	C	353	LEU
1	C	357	LYS
1	C	364	LEU
1	C	385	ARG
1	C	443	THR
1	C	462	GLN
1	D	34	LEU
1	D	58	THR
1	D	108	HIS
1	D	123	LEU
1	D	136	LEU
1	D	139	LEU
1	D	181	THR
1	D	245	PHE
1	D	248	LEU
1	D	283	LEU
1	D	325	LEU
1	D	364	LEU
1	D	375	LEU
1	D	407	LYS
1	D	408	LEU
1	D	443	THR
1	D	458	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	ASN
1	A	114	ASN
1	A	116	GLN
1	A	176	HIS
1	A	426	GLN
1	A	432	ASN
1	A	462	GLN
1	B	89	ASN
1	B	108	HIS
1	B	165	GLN
1	B	176	HIS
1	B	195	ASN
1	B	462	GLN

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Mol	Chain	Res	Type
1	C	89	ASN
1	C	108	HIS
1	C	160	HIS
1	C	165	GLN
1	C	286	GLN
1	C	436	GLN
1	D	127	ASN
1	D	165	GLN
1	D	207	ASN
1	D	322	ASN
1	D	436	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

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	447/468 (95%)	-0.61	5 (1%)	80 82	6, 23, 61, 87	0
1	B	447/468 (95%)	-0.60	7 (1%)	72 74	6, 24, 62, 87	0
1	C	447/468 (95%)	-0.41	6 (1%)	77 79	7, 33, 68, 83	0
1	D	447/468 (95%)	-0.55	4 (0%)	84 86	9, 29, 61, 84	0
All	All	1788/1872 (95%)	-0.54	22 (1%)	79 80	6, 27, 63, 87	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	460	LYS	3.5
1	C	462	GLN	3.4
1	C	463	LYS	3.3
1	B	463	LYS	2.9
1	B	17	THR	2.9
1	D	83	GLN	2.8
1	B	76	LYS	2.8
1	A	462	GLN	2.7
1	B	19	PRO	2.7
1	D	422	SER	2.6
1	A	285	PRO	2.5
1	B	281	SER	2.4
1	D	460	LYS	2.4
1	A	17	THR	2.3
1	A	385	ARG	2.2
1	B	82	LYS	2.1
1	D	76	LYS	2.1
1	C	82	LYS	2.1
1	C	76	LYS	2.1
1	B	286	GLN	2.0
1	C	411	GLU	2.0
1	A	282	SER	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.