Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 02:27 AM EDT

PDB ID	:	3R7S
Title	:	Crystal Structure of Apo Caspase2
Authors	:	Tang, Y.; Wells, J.; Arkin, M.
Deposited on	:	2011-03-22
Resolution	:	2.25 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:

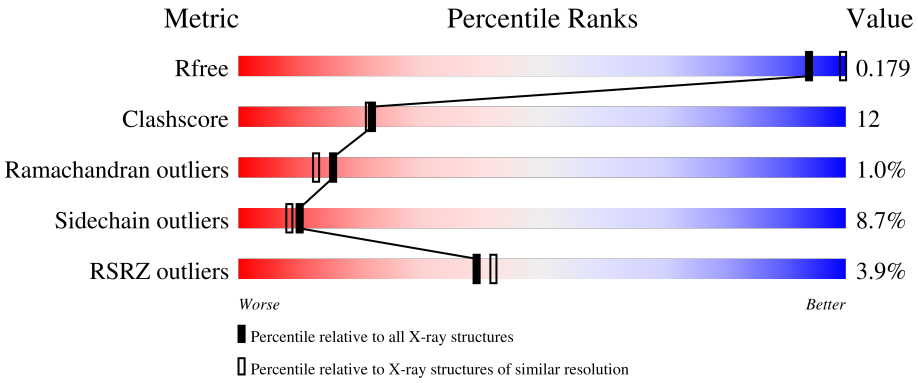
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	160	72% 21% 6%
1	C	160	74% 21%
2	B	112	12% 68% 18% 12%
2	D	112	3% 62% 19% 15%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4135 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-2 subunit p18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	159	Total	C	N	O	S	2	0	0
			1235	783	217	227	8			
1	C	159	Total	C	N	O	S	1	0	0
			1242	787	220	227	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	174	MET	-	EXPRESSION TAG	UNP P42575
C	174	MET	-	EXPRESSION TAG	UNP P42575

- Molecule 2 is a protein called Caspase-2 subunit p12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	98	Total	C	N	O	S	0	2	0
			765	480	139	132	14			
2	D	95	Total	C	N	O	S	0	2	0
			758	476	136	133	13			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	453	LEU	-	EXPRESSION TAG	UNP P42575
B	454	GLU	-	EXPRESSION TAG	UNP P42575
B	455	HIS	-	EXPRESSION TAG	UNP P42575
B	456	HIS	-	EXPRESSION TAG	UNP P42575
B	457	HIS	-	EXPRESSION TAG	UNP P42575
B	458	HIS	-	EXPRESSION TAG	UNP P42575
B	459	HIS	-	EXPRESSION TAG	UNP P42575
B	460	HIS	-	EXPRESSION TAG	UNP P42575
D	453	LEU	-	EXPRESSION TAG	UNP P42575
D	454	GLU	-	EXPRESSION TAG	UNP P42575

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Chain	Residue	Modelled	Actual	Comment	Reference
D	455	HIS	-	EXPRESSION TAG	UNP P42575
D	456	HIS	-	EXPRESSION TAG	UNP P42575
D	457	HIS	-	EXPRESSION TAG	UNP P42575
D	458	HIS	-	EXPRESSION TAG	UNP P42575
D	459	HIS	-	EXPRESSION TAG	UNP P42575
D	460	HIS	-	EXPRESSION TAG	UNP P42575

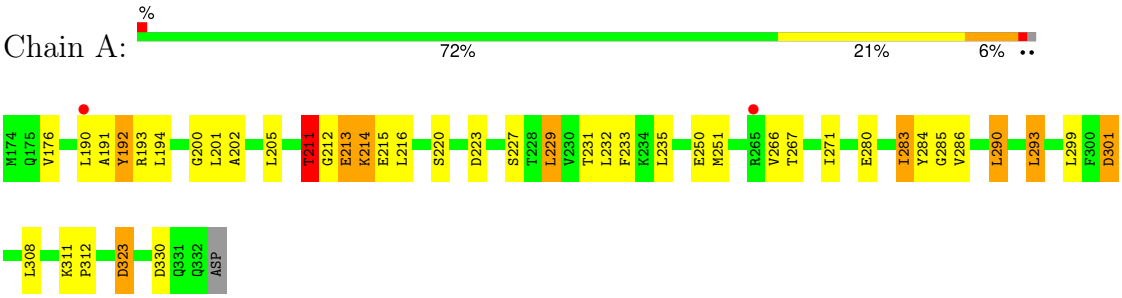
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	38	Total O 38 38	0	0
3	B	28	Total O 28 28	0	0
3	C	43	Total O 43 43	0	0
3	D	26	Total O 26 26	0	0

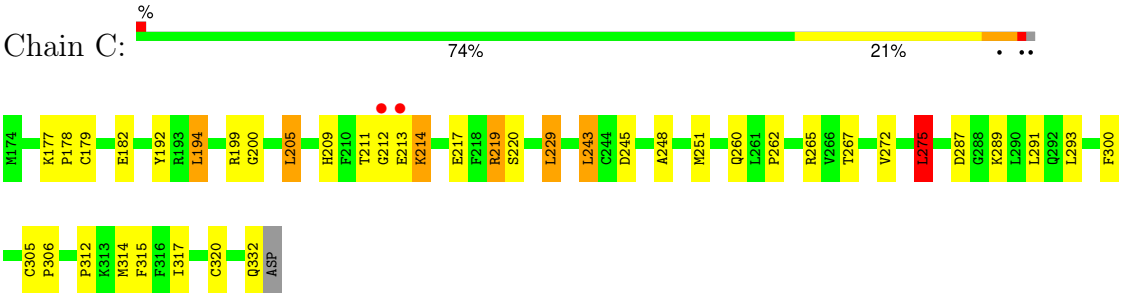
3 Residue-property plots (i)

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.

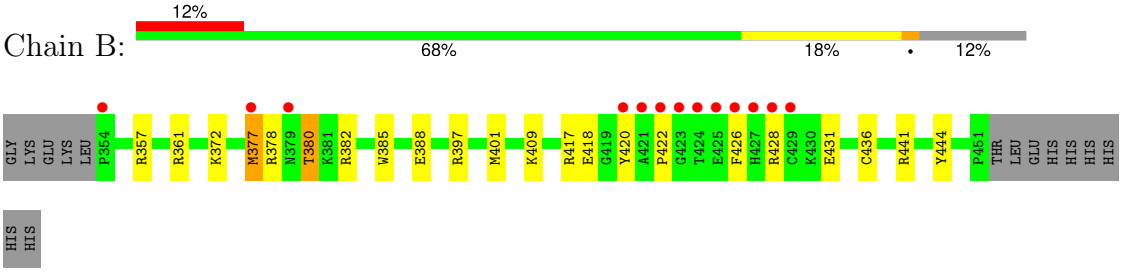
• Molecule 1: Caspase-2 subunit p18



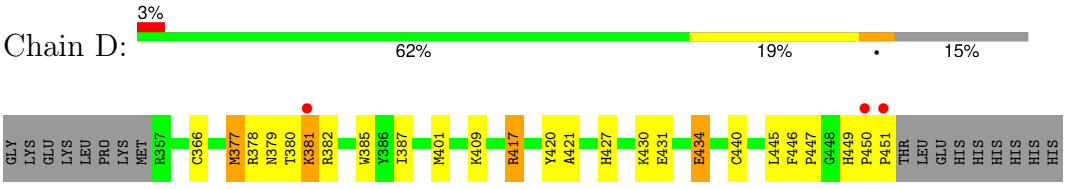
• Molecule 1: Caspase-2 subunit p18



• Molecule 2: Caspase-2 subunit p12



• Molecule 2: Caspase-2 subunit p12



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.16Å 82.81Å 112.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.55 – 2.25 49.55 – 2.25	Depositor EDS
% Data completeness (in resolution range)	95.2 (49.55-2.25) 99.6 (49.55-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.59 (at 2.25Å)	Xtriage
Refinement program	PHENIX 1.4_49, REFMAC 5.5.0109	Depositor
R, R_{free}	0.175 , 0.226 0.180 , 0.179	Depositor DCC
R_{free} test set	1681 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	37.8	Xtriage
Anisotropy	0.722	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 40.0	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	0.96	EDS
Total number of atoms	4135	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.04% 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	1.07	3/1260 (0.2%)	1.02	4/1706 (0.2%)
1	C	0.99	1/1267 (0.1%)	1.01	6/1714 (0.4%)
2	B	1.03	1/789 (0.1%)	0.98	1/1062 (0.1%)
2	D	1.11	2/782 (0.3%)	1.04	1/1053 (0.1%)
All	All	1.05	7/4098 (0.2%)	1.01	12/5535 (0.2%)

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

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	431	GLU	CG-CD	6.51	1.61	1.51
2	B	444	TYR	CD1-CE1	6.29	1.48	1.39
1	A	250	GLU	CG-CD	5.84	1.60	1.51
1	A	250	GLU	CB-CG	5.66	1.62	1.52
1	A	192	TYR	CD2-CE2	5.48	1.47	1.39
2	D	434	GLU	CG-CD	5.39	1.60	1.51
1	C	300	PHE	CE1-CZ	5.10	1.47	1.37

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	265	ARG	NE-CZ-NH1	-6.91	116.85	120.30
1	C	219	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	A	301	ASP	CB-CG-OD2	6.02	123.72	118.30
1	C	320	CYS	CA-CB-SG	-5.87	103.44	114.00
1	A	223	ASP	CB-CG-OD2	5.86	123.57	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	275	LEU	CA-CB-CG	5.48	127.90	115.30
1	C	219	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	C	314	MET	CG-SD-CE	-5.30	91.71	100.20
2	B	361	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	283	ILE	CB-CA-C	-5.18	101.23	111.60
2	D	440	CYS	CA-CB-SG	-5.15	104.73	114.00
1	A	293	LEU	CA-CB-CG	-5.14	103.48	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	211	THR	Peptide
1	A	214	LYS	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	1235	0	1203	34	0
1	C	1242	0	1216	33	0
2	B	765	0	751	15	0
2	D	758	0	749	23	1
3	A	38	0	0	3	0
3	B	28	0	0	1	0
3	C	43	0	0	5	1
3	D	26	0	0	2	0
All	All	4135	0	3919	93	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (93) 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:C:179:CYS:HB2	3:C:534:HOH:O	1.53	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:CYS:SG	3:C:534:HOH:O	2.20	0.98
1:C:179:CYS:CB	3:C:534:HOH:O	2.11	0.95
1:C:194:LEU:HD23	1:C:199:ARG:HD2	1.53	0.89
1:C:220:SER:HB2	2:D:380:THR:HG22	1.59	0.84
1:C:262:PRO:HG2	3:C:522:HOH:O	1.78	0.83
1:C:248:ALA:HA	1:C:251:MET:CE	2.11	0.80
1:C:220:SER:CB	2:D:380:THR:HG22	2.13	0.77
1:A:220:SER:O	2:B:378:ARG:HD2	1.86	0.76
1:A:211:THR:CG2	1:A:213:GLU:H	2.00	0.74
1:C:220:SER:O	2:D:378:ARG:HD2	1.87	0.74
1:C:194:LEU:CD2	1:C:199:ARG:HD2	2.17	0.74
1:A:212:GLY:C	1:A:214:LYS:H	1.93	0.71
2:B:377:MET:HG2	2:B:385:TRP:CZ2	2.25	0.70
1:A:211:THR:HG22	1:A:213:GLU:H	1.57	0.69
2:B:397:ARG:CZ	2:B:401:MET:HE1	2.25	0.66
2:D:377:MET:HA	2:D:377:MET:HE3	1.79	0.65
1:C:248:ALA:HA	1:C:251:MET:HE2	1.80	0.64
1:C:179:CYS:HB3	2:D:447:PRO:HD2	1.78	0.63
1:A:220:SER:OG	2:B:380:THR:HB	1.98	0.63
2:D:430:LYS:HE3	3:D:522:HOH:O	2.00	0.62
1:A:284:TYR:CD2	1:A:290:LEU:HD13	2.34	0.62
1:C:229:LEU:HD13	2:D:387:ILE:HG23	1.81	0.62
1:A:211:THR:HG22	1:A:213:GLU:N	2.16	0.61
2:D:401:MET:SD	2:D:409:LYS:HD2	2.40	0.61
1:A:212:GLY:C	1:A:214:LYS:N	2.54	0.61
1:C:211:THR:O	1:C:213:GLU:N	2.33	0.60
2:B:382:ARG:HH21	2:B:388:GLU:CD	2.04	0.60
1:A:212:GLY:HA3	3:A:507:HOH:O	1.99	0.60
1:A:211:THR:HB	1:A:286:VAL:O	2.03	0.58
2:B:357:ARG:HD3	3:B:511:HOH:O	2.02	0.58
2:D:385:TRP:CE3	2:D:417:ARG:HG2	2.39	0.57
1:C:220:SER:OG	2:D:380:THR:HG22	2.04	0.56
1:C:213:GLU:O	1:C:214:LYS:HB2	2.06	0.56
1:C:214:LYS:O	1:C:214:LYS:HG3	2.07	0.55
1:C:209:HIS:HD2	1:C:245:ASP:OD2	1.89	0.54
1:A:212:GLY:CA	3:A:507:HOH:O	2.55	0.53
1:A:211:THR:HG23	1:A:213:GLU:H	1.73	0.53
1:A:308:LEU:O	1:A:311:LYS:HB2	2.08	0.53
1:A:201:LEU:HD23	1:A:201:LEU:N	2.24	0.52
1:A:205:LEU:C	1:A:205:LEU:HD23	2.30	0.52
1:A:323:ASP:OD1	1:A:323:ASP:N	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:TYR:CD1	1:A:312:PRO:HD3	2.46	0.49
1:C:205:LEU:C	1:C:205:LEU:HD13	2.31	0.49
2:D:446:PHE:N	2:D:447:PRO:HD3	2.28	0.49
2:B:397:ARG:HB3	2:B:401:MET:HE3	1.94	0.48
1:A:200:GLY:HA2	1:A:267:THR:HB	1.96	0.48
1:A:212:GLY:O	1:A:214:LYS:N	2.48	0.47
1:C:192:TYR:CD1	1:C:312:PRO:HD3	2.49	0.47
2:D:377:MET:HB2	2:D:385:TRP:CE2	2.49	0.47
2:B:377:MET:HG2	2:B:385:TRP:CH2	2.49	0.46
1:A:280:GLU:HG2	2:B:372:LYS:NZ	2.30	0.46
1:C:275:LEU:N	1:C:275:LEU:HD23	2.30	0.46
1:A:231:THR:O	1:A:235:LEU:HG	2.15	0.46
2:D:377:MET:HG3	2:D:385:TRP:CH2	2.51	0.46
1:C:205:LEU:C	1:C:205:LEU:CD1	2.84	0.46
1:A:251:MET:CE	1:A:285:GLY:HA2	2.46	0.45
1:A:301:ASP:C	1:A:301:ASP:OD1	2.55	0.45
1:C:219:ARG:NH2	3:C:529:HOH:O	2.19	0.45
1:A:191:ALA:O	2:B:441:ARG:NH1	2.50	0.45
2:D:385:TRP:CD2	2:D:417:ARG:HG2	2.52	0.45
1:A:212:GLY:HA2	3:A:512:HOH:O	2.16	0.45
1:C:205:LEU:HD22	1:C:243:LEU:HB3	1.98	0.45
1:A:284:TYR:CE2	1:A:290:LEU:HD13	2.52	0.45
1:C:177:LYS:HA	1:C:178:PRO:HD3	1.82	0.45
1:C:317:ILE:HD13	2:D:366[C]:CYS:SG	2.57	0.45
1:C:200:GLY:HA2	1:C:267:THR:HB	1.99	0.44
2:B:397:ARG:NH2	2:B:401:MET:HE1	2.32	0.44
2:D:382:ARG:NH1	3:D:518:HOH:O	2.51	0.44
2:D:421:ALA:O	2:D:427:HIS:HB2	2.18	0.44
2:B:436[B]:CYS:SG	2:D:434:GLU:OE1	2.76	0.44
1:A:202:ALA:HA	1:A:271:ILE:O	2.18	0.44
1:A:308:LEU:HA	1:A:311:LYS:HD2	2.00	0.43
2:D:381:LYS:HB3	2:D:381:LYS:HE2	1.31	0.43
2:D:449:HIS:HA	2:D:450:PRO:C	2.40	0.42
2:D:450:PRO:HA	2:D:451:PRO:HD3	1.80	0.42
2:D:377:MET:HA	2:D:377:MET:CE	2.47	0.42
2:B:397:ARG:CZ	2:B:401:MET:CE	2.96	0.42
1:A:251:MET:CE	1:A:285:GLY:CA	2.98	0.42
2:D:377:MET:HB2	2:D:385:TRP:CD2	2.54	0.42
2:B:420:TYR:CD2	2:B:422:PRO:HD3	2.55	0.42
1:C:275:LEU:N	1:C:275:LEU:CD2	2.82	0.42
1:C:293:LEU:HD23	1:C:293:LEU:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:CYS:N	1:C:306:PRO:HD3	2.35	0.42
1:A:293:LEU:HD23	1:A:293:LEU:HA	1.89	0.41
1:A:251:MET:HE2	1:A:285:GLY:CA	2.51	0.41
1:A:251:MET:HE2	1:A:285:GLY:HA2	2.01	0.41
1:C:272:VAL:O	1:C:315:PHE:HA	2.21	0.41
1:C:248:ALA:HA	1:C:251:MET:HE3	1.97	0.41
1:C:287:ASP:N	1:C:287:ASP:OD1	2.53	0.41
2:B:420:TYR:HD2	2:B:420:TYR:O	2.03	0.41
1:A:193:ARG:HE	1:A:193:ARG:HB3	1.46	0.40
1:A:229:LEU:HG	1:A:233:PHE:CE2	2.55	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:420:TYR:OH	3:C:513:HOH:O[4_455]	2.09	0.11

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	157/160 (98%)	148 (94%)	7 (4%)	2 (1%)	12 8
1	C	157/160 (98%)	150 (96%)	5 (3%)	2 (1%)	12 8
2	B	98/112 (88%)	94 (96%)	3 (3%)	1 (1%)	15 13
2	D	95/112 (85%)	93 (98%)	2 (2%)	0	100 100
All	All	507/544 (93%)	485 (96%)	17 (3%)	5 (1%)	15 13

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	213	GLU
1	A	215	GLU
2	B	426	PHE
1	C	212	GLY
1	C	214	LYS

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	133/140 (95%)	119 (90%)	14 (10%)	7 5
1	C	134/140 (96%)	123 (92%)	11 (8%)	11 10
2	B	81/96 (84%)	74 (91%)	7 (9%)	10 9
2	D	82/96 (85%)	77 (94%)	5 (6%)	18 18
All	All	430/472 (91%)	393 (91%)	37 (9%)	10 9

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	VAL
1	A	190	LEU
1	A	194	LEU
1	A	211	THR
1	A	216	LEU
1	A	227	SER
1	A	229	LEU
1	A	232	LEU
1	A	266	VAL
1	A	283	ILE
1	A	290	LEU
1	A	299	LEU
1	A	323	ASP
1	A	330	ASP
2	B	377	MET
2	B	380	THR
2	B	409	LYS

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Mol	Chain	Res	Type
2	B	417	ARG
2	B	418	GLU
2	B	428	ARG
2	B	431	GLU
1	C	182	GLU
1	C	194	LEU
1	C	205	LEU
1	C	217	GLU
1	C	229	LEU
1	C	243	LEU
1	C	260	GLN
1	C	275	LEU
1	C	289	LYS
1	C	291	LEU
1	C	332	GLN
2	D	377	MET
2	D	379	ASN
2	D	381	LYS
2	D	417	ARG
2	D	445	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	HIS
1	C	195	GLN
1	C	209	HIS
1	C	257	ASN
2	D	449	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	159/160 (99%)	-0.28	2 (1%) 77 79	30, 41, 66, 79	3 (1%)
1	C	159/160 (99%)	-0.34	2 (1%) 77 79	28, 41, 66, 93	1 (0%)
2	B	98/112 (87%)	0.32	13 (13%) 3 3	26, 42, 92, 108	0
2	D	95/112 (84%)	-0.20	3 (3%) 47 50	25, 40, 67, 72	0
All	All	511/544 (93%)	-0.17	20 (3%) 39 42	25, 41, 71, 108	4 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	424	THR	6.4
2	B	423	GLY	5.9
2	B	420	TYR	5.7
2	B	425	GLU	5.0
2	B	422	PRO	4.3
2	B	421	ALA	4.2
2	D	451	PRO	4.0
2	B	354	PRO	3.9
2	B	426	PHE	3.3
2	D	450	PRO	3.2
2	B	429	CYS	2.8
1	C	212	GLY	2.8
2	B	377	MET	2.5
2	B	427	HIS	2.5
1	C	213	GLU	2.3
2	B	428	ARG	2.3
2	D	381	LYS	2.1
2	B	379	ASN	2.0
1	A	265	ARG	2.0
1	A	190	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.