



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 12:25 pm GMT

PDB ID : 4JJ8
Title : Caspase-3 specific unnatural amino acid peptides
Authors : Vickers, C.J.; Gonzalez-Paez, G.E.; Wolan, D.W.
Deposited on : 2013-03-07
Resolution : 2.94 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

<http://wwpdb.org/validation/2016/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
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

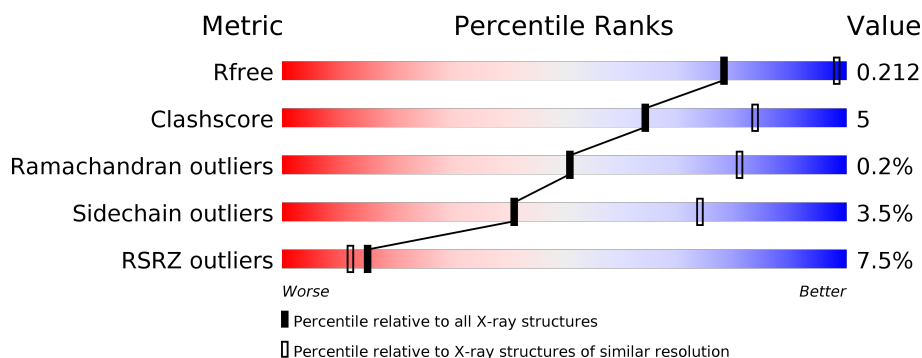
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.94 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}	100719	2289 (2.98-2.90)
Clashscore	112137	2543 (2.98-2.90)
Ramachandran outliers	110173	2475 (2.98-2.90)
Sidechain outliers	110143	2477 (2.98-2.90)
RSRZ outliers	101464	2301 (2.98-2.90)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$. 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	255	<div> <div>8%</div> <div> <div></div> <div>80%</div> <div>9%</div> <div>9%</div> </div> </div>
1	B	255	<div> <div>5%</div> <div> <div></div> <div>75%</div> <div>15%</div> <div>9%</div> </div> </div>
2	C	6	<div> <div>17%</div> <div> <div></div> <div>83%</div> <div>17%</div> </div> </div>
2	D	6	<div> <div>17%</div> <div> <div></div> <div>67%</div> <div>33%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3783 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-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	0	0
			1825	1157	309	344	15			
1	B	231	Total	C	N	O	S	0	0	0
			1822	1160	309	338	15			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	304	GLN	-	EXPRESSION TAG	UNP P55210
A	305	LEU	-	EXPRESSION TAG	UNP P55210
A	306	HIS	-	EXPRESSION TAG	UNP P55210
A	307	HIS	-	EXPRESSION TAG	UNP P55210
A	308	HIS	-	EXPRESSION TAG	UNP P55210
A	309	HIS	-	EXPRESSION TAG	UNP P55210
A	310	HIS	-	EXPRESSION TAG	UNP P55210
A	311	HIS	-	EXPRESSION TAG	UNP P55210
B	304	GLN	-	EXPRESSION TAG	UNP P55210
B	305	LEU	-	EXPRESSION TAG	UNP P55210
B	306	HIS	-	EXPRESSION TAG	UNP P55210
B	307	HIS	-	EXPRESSION TAG	UNP P55210
B	308	HIS	-	EXPRESSION TAG	UNP P55210
B	309	HIS	-	EXPRESSION TAG	UNP P55210
B	310	HIS	-	EXPRESSION TAG	UNP P55210
B	311	HIS	-	EXPRESSION TAG	UNP P55210

- Molecule 2 is a protein called Caspase Inhibitor.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	6	Total	C	N	O	0	0	0
			49	33	6	10			
2	D	6	Total	C	N	O	0	0	0
			49	33	6	10			

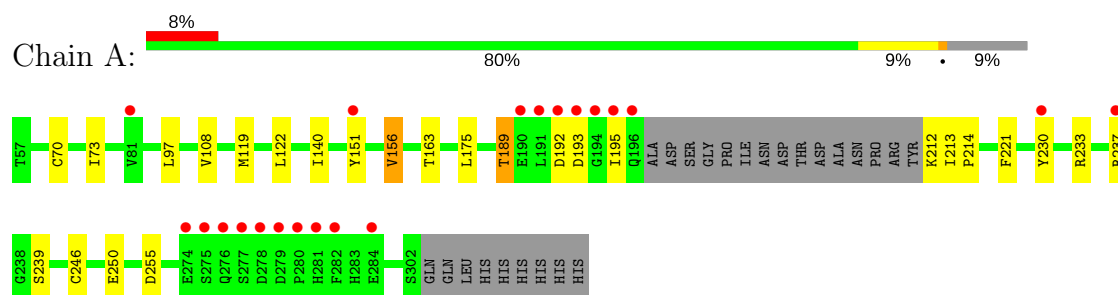
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	14	Total 14	O 14	0	0
3	B	24	Total 24	O 24	0	0

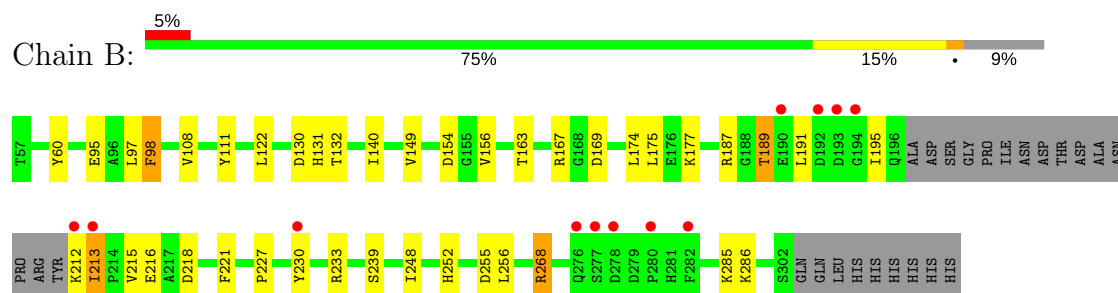
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

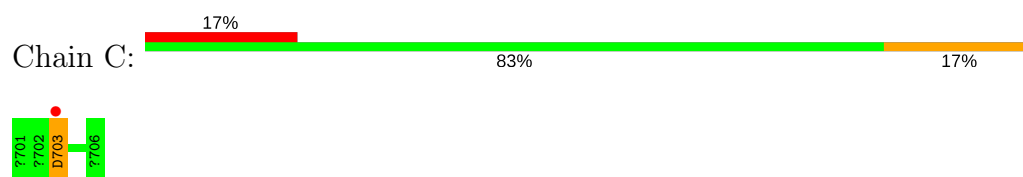
• Molecule 1: Caspase-7



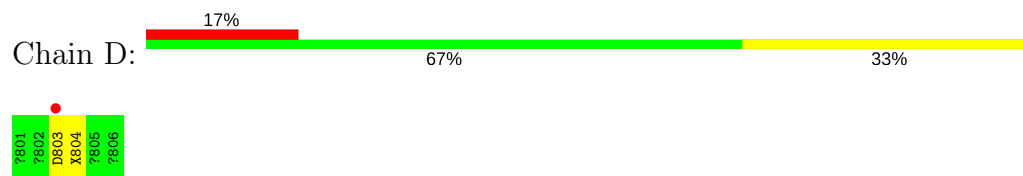
• Molecule 1: Caspase-7



• Molecule 2: Caspase Inhibitor



• Molecule 2: Caspase Inhibitor



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	89.09Å 89.09Å 185.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.26 – 2.94 48.26 – 2.94	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.26-2.94) 100.0 (48.26-2.94)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.96Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.193 , 0.216 0.189 , 0.212	Depositor DCC
R_{free} test set	969 reflections (5.14%)	DCC
Wilson B-factor (Å ²)	73.9	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3783	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: B3L, 1U8, 1MH, ACE, HLX

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	0.25	0/1864	0.43	0/2515
1	B	0.25	0/1861	0.44	0/2508
2	C	0.18	0/7	0.61	0/8
2	D	0.17	0/7	0.44	0/8
All	All	0.25	0/3739	0.44	0/5039

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
2	C	0	1
2	D	0	3
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	703	ASP	Peptide
2	D	803	ASP	Peptide
2	D	804	B3L	Mainchain,Peptide

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	1825	0	1748	16	0
1	B	1822	0	1770	26	0
2	C	49	0	42	0	0
2	D	49	0	41	0	0
3	A	14	0	0	0	0
3	B	24	0	0	0	0
All	All	3783	0	3601	35	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 5.

All (35) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ASP:O	1:B:212:LYS:NZ	2.25	0.68
1:A:163:THR:HG21	1:A:221:PHE:HE2	1.60	0.66
1:B:163:THR:HG21	1:B:221:PHE:HE2	1.63	0.62
1:B:97:LEU:HD13	1:B:140:ILE:HG21	1.83	0.59
1:A:233:ARG:HA	1:A:239:SER:HA	1.83	0.59
1:A:195:ILE:HD11	1:B:175:LEU:HD11	1.88	0.55
1:A:175:LEU:HG	1:A:213:ILE:HD11	1.88	0.54
1:B:233:ARG:HA	1:B:239:SER:HA	1.89	0.53
1:B:167:ARG:HG2	1:B:215:VAL:HB	1.91	0.53
1:A:70:CYS:HB3	1:A:108:VAL:HG22	1.92	0.51
1:A:97:LEU:HD13	1:A:140:ILE:HG21	1.92	0.51
1:A:195:ILE:N	1:B:212:LYS:HD2	2.26	0.51
1:A:151:TYR:CE1	1:A:156:VAL:HG12	2.44	0.51
1:B:175:LEU:HD21	1:B:213:ILE:HD11	1.93	0.50
1:B:248:ILE:HD11	1:B:268:ARG:HG3	1.94	0.49
1:A:189:THR:HA	1:A:230:TYR:CE1	2.47	0.49
1:B:191:LEU:HD23	1:B:285:LYS:HG3	1.95	0.48
1:A:192:ASP:OD1	1:B:215:VAL:HG22	2.14	0.47
1:B:130:ASP:OD1	1:B:132:THR:OG1	2.22	0.47
1:B:189:THR:HA	1:B:230:TYR:CE1	2.49	0.46
1:B:131:HIS:O	1:B:177:LYS:NZ	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ILE:HD11	1:B:175:LEU:CD1	2.47	0.45
1:B:175:LEU:HD12	1:B:175:LEU:HA	1.58	0.45
1:B:169:ASP:OD1	1:B:169:ASP:N	2.49	0.44
1:B:174:LEU:HA	1:B:177:LYS:HD2	1.99	0.44
1:B:95:GLU:HA	1:B:98:PHE:HD2	1.83	0.44
1:A:246:CYS:O	1:A:250:GLU:HG3	2.17	0.44
1:A:73:ILE:HD13	1:A:119:MET:HG2	2.00	0.43
1:B:215:VAL:HG23	1:B:216:GLU:HG2	2.00	0.42
1:A:214:PRO:HG3	1:B:286:LYS:HB3	2.02	0.42
1:B:60:TYR:OH	1:B:218:ASP:OD1	2.19	0.41
1:B:252:HIS:HB3	1:B:256:LEU:HG	2.03	0.41
1:B:111:TYR:CG	1:B:122:LEU:HD11	2.56	0.41
1:B:187:ARG:CZ	1:B:227:PRO:HG3	2.51	0.40
1:A:212:LYS:HA	1:B:195:ILE:O	2.21	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	227/255 (89%)	225 (99%)	2 (1%)	0	100	100
1	B	227/255 (89%)	224 (99%)	3 (1%)	0	100	100
2	C	1/6 (17%)	0	0	1 (100%)	0	0
2	D	1/6 (17%)	1 (100%)	0	0	100	100
All	All	456/522 (87%)	450 (99%)	5 (1%)	1 (0%)	51	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	703	ASP

5.3.2 Protein sidechains ⓘ

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	197/224 (88%)	192 (98%)	5 (2%)	53	82
1	B	197/224 (88%)	188 (95%)	9 (5%)	31	64
2	C	1/1 (100%)	1 (100%)	0	100	100
2	D	1/1 (100%)	1 (100%)	0	100	100
All	All	396/450 (88%)	382 (96%)	14 (4%)	41	74

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	LEU
1	A	156	VAL
1	A	189	THR
1	A	237	ARG
1	A	255	ASP
1	B	98	PHE
1	B	108	VAL
1	B	149	VAL
1	B	154	ASP
1	B	156	VAL
1	B	189	THR
1	B	213	ILE
1	B	255	ASP
1	B	268	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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$
2	1MH	C	702	2	11,11,12	0.46	0	11,13,15	1.56	2 (18%)
2	B3L	C	704	2	8,8,9	0.46	0	8,9,11	1.00	1 (12%)
2	HLX	C	705	2	8,8,9	0.52	0	6,9,11	1.06	0
2	1U8	C	706	1,2	4,8,20	0.42	0	2,10,27	0.47	0
2	1MH	D	802	2	11,11,12	0.49	0	11,13,15	1.51	2 (18%)
2	B3L	D	804	2	8,8,9	0.48	0	8,9,11	1.29	2 (25%)
2	HLX	D	805	2	8,8,9	0.55	0	6,9,11	1.08	0
2	1U8	D	806	1,2	4,8,20	0.43	0	2,10,27	0.63	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	1MH	C	702	2	-	0/4/6/8	0/1/1/1
2	B3L	C	704	2	-	0/7/7/8	0/0/0/0
2	HLX	C	705	2	-	0/5/7/9	0/0/0/0
2	1U8	C	706	1,2	-	0/5/8/17	0/0/0/1
2	1MH	D	802	2	-	0/4/6/8	0/1/1/1
2	B3L	D	804	2	-	0/7/7/8	0/0/0/0
2	HLX	D	805	2	-	0/5/7/9	0/0/0/0
2	1U8	D	806	1,2	-	0/5/8/17	0/0/0/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	702	1MH	C6-CB-CA	-2.74	108.77	114.29
2	D	802	1MH	C6-CB-CA	-2.54	109.17	114.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	804	B3L	CD-CG-CB	-2.20	109.75	116.62
2	C	704	B3L	O-C-CA	-2.05	118.85	125.48
2	D	804	B3L	O-C-CA	-2.01	118.96	125.48
2	C	702	1MH	C9-N8-C7	2.47	121.16	116.83
2	D	802	1MH	C9-N8-C7	2.50	121.21	116.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	231/255 (90%)	0.36	21 (9%) 10 8	19, 45, 99, 142	0
1	B	231/255 (90%)	0.27	12 (5%) 28 26	20, 41, 99, 139	0
2	C	1/6 (16%)	2.85	1 (100%) 0 0	97, 97, 97, 97	0
2	D	1/6 (16%)	2.54	1 (100%) 0 0	101, 101, 101, 101	0
All	All	464/522 (88%)	0.33	35 (7%) 15 12	19, 43, 99, 142	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	278	ASP	7.8
1	A	194	GLY	5.7
1	B	280	PRO	5.5
1	A	276	GLN	5.0
1	A	277	SER	4.5
1	A	282	PHE	4.3
1	B	278	ASP	4.2
1	A	281	HIS	3.4
1	A	81	VAL	3.2
1	A	280	PRO	3.1
1	A	275	SER	3.1
1	B	282	PHE	3.1
1	B	192	ASP	2.9
2	C	703	ASP	2.9
1	A	195	ILE	2.8
1	A	192	ASP	2.8
1	A	190	GLU	2.7
1	A	191	LEU	2.7
1	A	274	GLU	2.6
1	B	277	SER	2.6
2	D	803	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	230	TYR	2.5
1	B	230	TYR	2.5
1	B	194	GLY	2.5
1	B	276	GLN	2.5
1	A	279	ASP	2.4
1	B	212	LYS	2.3
1	A	193	ASP	2.3
1	A	151	TYR	2.3
1	A	196	GLN	2.2
1	B	193	ASP	2.2
1	B	190	GLU	2.1
1	A	237	ARG	2.1
1	B	213	ILE	2.1
1	A	284	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	1MH	D	802	11/12	0.84	0.56	-	78,102,115,118	0
2	1U8	C	706	9/20	0.94	0.20	-	55,68,80,83	0
2	HLX	D	805	9/10	0.95	0.30	-	39,44,57,70	0
2	1MH	C	702	11/12	0.86	0.52	-	86,109,121,123	0
2	1U8	D	806	9/20	0.92	0.19	-	40,49,69,74	0
2	HLX	C	705	9/10	0.98	0.47	-	62,77,86,87	0
2	B3L	D	804	9/10	0.89	0.47	-	57,66,88,108	0
2	B3L	C	704	9/10	0.92	0.56	-	55,76,89,90	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.