Full wwPDB X-ray Structure Validation Report (i)

Nov 7, 2023 – 09:06 AM EST

PDB ID	:	6U3I
Title	:	Design of organo-peptides as bipartite PCSK9 antagonists
Authors	:	Ultsch, M.H.; Kirchhofer, D.
Deposited on	:	2019-08-21
Resolution	:	2.90 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 (i) 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 (i)) were used in the production of this report:

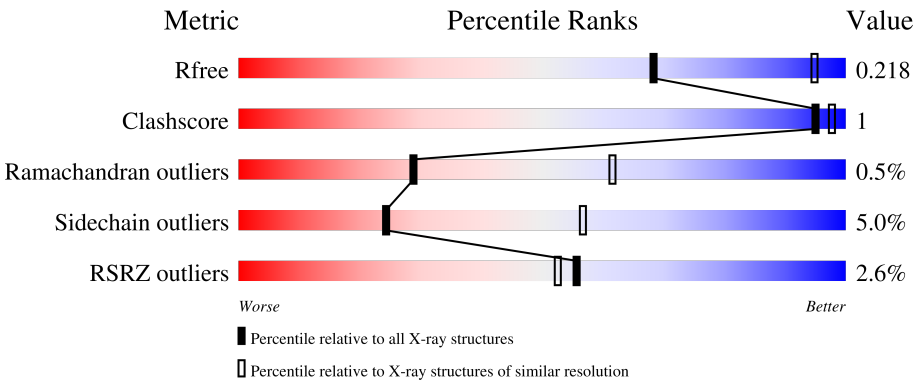
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 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	700	2%, 78%, 5%, 17%
2	B	11	9%, 82%, 18%
3	H	223	3%, 89%, 9%
4	L	214	3%, 94%, 6%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 15452 atoms, of which 7599 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 Proprotein convertase subtilisin/kexin type 9.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	582	8662	2708	4295	808	817	34	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	474	ILE	VAL	variant	UNP Q8NBP7
A	670	GLU	GLY	variant	UNP Q8NBP7
A	693	HIS	-	expression tag	UNP Q8NBP7
A	694	HIS	-	expression tag	UNP Q8NBP7
A	695	HIS	-	expression tag	UNP Q8NBP7
A	696	HIS	-	expression tag	UNP Q8NBP7
A	697	HIS	-	expression tag	UNP Q8NBP7
A	698	HIS	-	expression tag	UNP Q8NBP7
A	699	HIS	-	expression tag	UNP Q8NBP7
A	700	HIS	-	expression tag	UNP Q8NBP7

- Molecule 2 is a protein called cis-1-amino-4-phenylcyclohexaneacyl-WNLK(hR)I(D-ser)LLR - NH2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
2	B	11	225	74	118	20	13	0	0	0

- Molecule 3 is a protein called 7G7 heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	H	222	3300	1075	1609	271	338	7	0	0	0

- Molecule 4 is a protein called 7G7 light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
4	L	214	3238	1035	1577	278	340	8	0	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
5	A	1	1	1	0	0

- Molecule 6 is water.

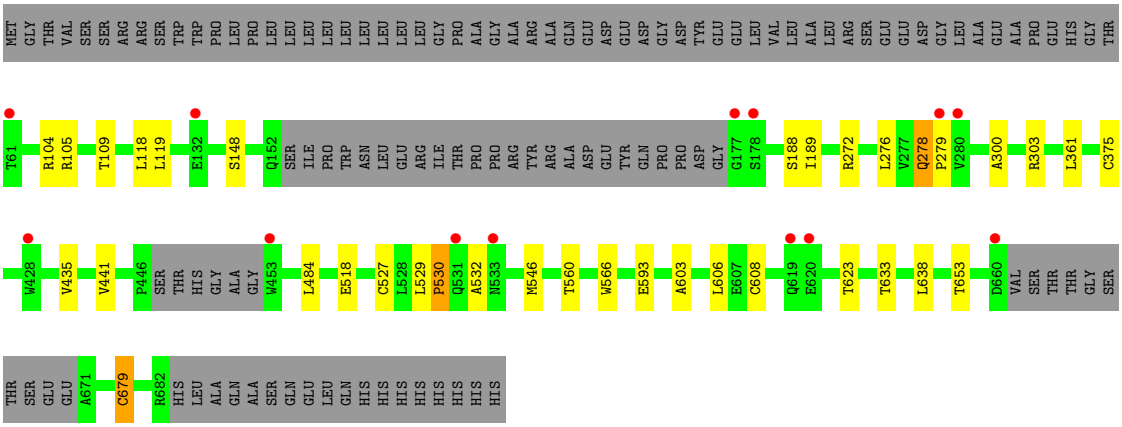
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	20	20	20	0	0
6	B	1	1	1	0	0
6	H	1	1	1	0	0
6	L	4	4	4	0	0

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: Proprotein convertase subtilisin/kexin type 9

Chain A:

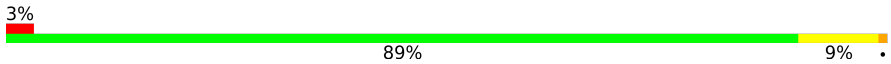


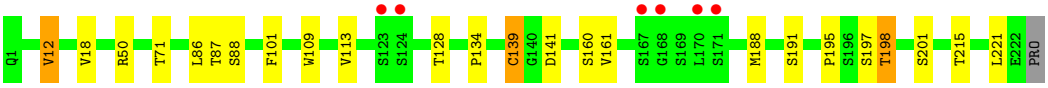
- Molecule 2: cis-1-amino-4-phenylcyclohexaneacyl-WNLK(hR)I(D-ser)LLR - NH2

Chain B:

- Molecule 3: 7G7 heavy chain

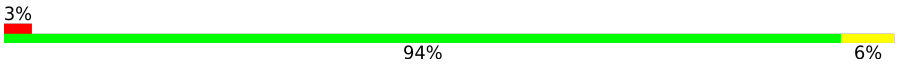
Chain H:

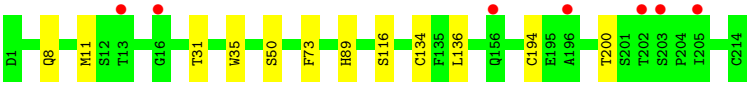




- Molecule 4: 7G7 light chain

Chain L:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	111.57Å 143.03Å 241.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.20 – 2.90 48.20 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.20-2.90) 99.9 (48.20-2.90)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 2.91Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.179 , 0.217 0.182 , 0.218	Depositor DCC
R_{free} test set	2197 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	55.1	Xtriage
Anisotropy	0.673	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 48.3	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	0.94	EDS
Total number of atoms	15452	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PQG, DSN, CA, HRG

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	0.53	0/4453	0.70	0/6045
2	B	0.41	0/73	0.53	0/94
3	H	0.49	0/1738	0.70	0/2375
4	L	0.50	0/1698	0.68	0/2301
All	All	0.52	0/7962	0.70	0/10815

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1	PQG	Mainchain

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	4367	4295	4297	12	0
2	B	107	118	103	1	0
3	H	1691	1609	1629	5	0
4	L	1661	1577	1580	2	0
5	A	1	0	0	0	0
6	A	20	0	0	0	0
6	B	1	0	0	0	0
6	H	1	0	0	0	0
6	L	4	0	0	0	0
All	All	7853	7599	7609	19	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 1.

All (19) 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:441:VAL:HG11	2:B:6:HRG:HD2	1.83	0.60
1:A:278:GLN:HB3	1:A:279:PRO:CD	2.35	0.57
1:A:560:THR:HB	1:A:633:THR:HG21	1.89	0.54
3:H:12:VAL:HG11	3:H:18:VAL:HG13	1.90	0.54
3:H:18:VAL:HG22	3:H:86:LEU:HD11	1.93	0.50
1:A:603:ALA:HB3	1:A:606:LEU:HB2	1.95	0.48
3:H:134:PRO:HB2	3:H:221:LEU:HD23	1.96	0.47
1:A:566:TRP:CZ3	1:A:593:GLU:HB2	2.50	0.47
1:A:278:GLN:CB	1:A:279:PRO:CD	2.94	0.46
3:H:101:PHE:CD2	3:H:109:TRP:HB3	2.51	0.46
3:H:195:PRO:HG2	3:H:198:THR:HG23	1.99	0.45
1:A:606:LEU:HD11	1:A:679:CYS:SG	2.58	0.43
1:A:529:LEU:HD23	1:A:532:ALA:CB	2.49	0.42
1:A:118:LEU:HD21	1:A:300:ALA:HB1	2.01	0.42
4:L:35:TRP:CE2	4:L:73:PHE:HB2	2.54	0.42
1:A:529:LEU:HD23	1:A:532:ALA:HB2	2.02	0.42
4:L:136:LEU:N	4:L:136:LEU:HD12	2.35	0.41
1:A:623:THR:HG23	1:A:653:THR:HG23	2.03	0.41
1:A:484:LEU:HD22	1:A:527:CYS:HB2	2.02	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	574/700 (82%)	538 (94%)	34 (6%)	2 (0%)	41	71
2	B	7/11 (64%)	7 (100%)	0	0	100	100
3	H	220/223 (99%)	212 (96%)	5 (2%)	3 (1%)	11	36
4	L	212/214 (99%)	207 (98%)	5 (2%)	0	100	100
All	All	1013/1148 (88%)	964 (95%)	44 (4%)	5 (0%)	29	61

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	278	GLN
1	A	530	PRO
3	H	139	CYS
3	H	160	SER
3	H	198	THR

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	468/566 (83%)	449 (96%)	19 (4%)	30	64
2	B	8/8 (100%)	8 (100%)	0	100	100
3	H	192/193 (100%)	177 (92%)	15 (8%)	12	34
4	L	189/189 (100%)	180 (95%)	9 (5%)	25	58
All	All	857/956 (90%)	814 (95%)	43 (5%)	24	57

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	ARG
1	A	105	ARG
1	A	109	THR
1	A	119	LEU
1	A	148	SER
1	A	188	SER
1	A	189	ILE
1	A	272	ARG
1	A	276	LEU
1	A	303	ARG
1	A	361	LEU
1	A	375	CYS
1	A	435	VAL
1	A	518	GLU
1	A	530	PRO
1	A	546	MET
1	A	608	CYS
1	A	638	LEU
1	A	679	CYS
3	H	12	VAL
3	H	50	ARG
3	H	71	THR
3	H	87	THR
3	H	88	SER
3	H	113	VAL
3	H	128	THR
3	H	139	CYS
3	H	141	ASP
3	H	161	VAL
3	H	188	MET
3	H	191	SER
3	H	197	SER
3	H	201	SER
3	H	215	THR
4	L	8	GLN
4	L	11	MET
4	L	31	THR
4	L	50	SER
4	L	89	HIS
4	L	116	SER
4	L	134	CYS
4	L	194	CYS

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Mol	Chain	Res	Type
4	L	200	THR

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

3 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	HRG	B	6	2	10,11,12	2.01	1 (10%)	6,12,14	0.83	0
2	PQG	B	1	2	12,16,17	0.72	0	15,22,24	2.09	3 (20%)

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	HRG	B	6	2	-	1/9/10/12	-
2	PQG	B	1	2	-	1/6/19/22	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	6	HRG	CZ-NE	5.92	1.45	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	PQG	C95-CA-C99	-5.06	100.44	108.41
2	B	1	PQG	C-CA-N	-4.90	99.04	109.35
2	B	1	PQG	C95-C96-C97	-2.87	108.65	111.37

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	6	HRG	NE-CD-CG-CG'
2	B	1	PQG	O-C-CA-C99

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	6	HRG	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	582/700 (83%)	0.18	13 (2%)	62	59	33, 51, 83, 112	0
2	B	8/11 (72%)	0.97	1 (12%)	3	3	45, 55, 77, 117	0
3	H	222/223 (99%)	0.42	6 (2%)	54	50	36, 62, 89, 105	0
4	L	214/214 (100%)	0.35	7 (3%)	46	41	37, 57, 82, 101	0
All	All	1026/1148 (89%)	0.27	27 (2%)	56	52	33, 55, 86, 117	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	171	SER	6.2
1	A	280	VAL	5.9
2	B	11	ARG	4.9
4	L	202	THR	3.3
1	A	531	GLN	3.1
4	L	205	ILE	2.9
3	H	124	SER	2.9
1	A	533	ASN	2.9
1	A	61	THR	2.8
4	L	16	GLY	2.7
3	H	123	SER	2.7
1	A	660	ASP	2.7
3	H	168	GLY	2.7
3	H	167	SER	2.6
4	L	203	SER	2.6
1	A	428	TRP	2.6
1	A	620	GLU	2.4
4	L	13	THR	2.4
4	L	196	ALA	2.3
1	A	453	TRP	2.3
1	A	132	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	177	GLY	2.3
1	A	619	GLN	2.2
1	A	178	SER	2.2
4	L	156	GLN	2.2
3	H	170	LEU	2.0
1	A	279	PRO	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. 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	B-factors(Å^2)	Q<0.9
2	HRG	B	6	12/13	0.95	0.25	39,47,51,57	0
2	DSN	B	8	6/7	0.95	0.13	55,57,60,61	0
2	PQG	B	1	15/16	0.97	0.30	50,59,69,70	0

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, 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	B-factors(Å^2)	Q<0.9
5	CA	A	801	1/1	0.88	0.17	83,83,83,83	0

6.5 Other polymers (i)

There are no such residues in this entry.