



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2018 – 01:54 PM EST

PDB ID : 5Q19
Title : Ligand binding to FARNESOID-X-RECEPTOR
Authors : Rudolph, M.G.; Benz, J.; Burger, D.; Thoma, R.; Ruf, A.; Joseph, C.; Kuhn, B.; Shao, C.; Yang, H.; Burley, S.K.
Deposited on : 2017-05-31
Resolution : 1.98 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 : rb-20030736
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) : rb-20030736

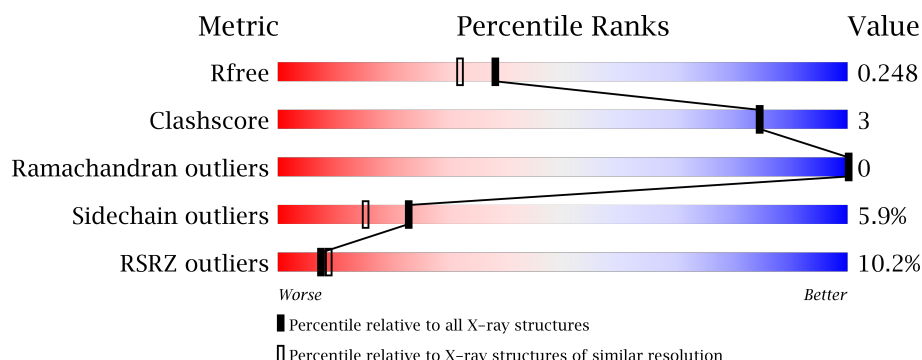
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	9293 (2.00-1.96)
Clashscore	112137	10621 (2.00-1.96)
Ramachandran outliers	110173	10502 (2.00-1.96)
Sidechain outliers	110143	10501 (2.00-1.96)
RSRZ outliers	101464	9395 (2.00-1.96)

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	233	<div> <div>9%</div> <div>87%</div> <div>10%</div> <div>..</div> </div>
1	C	233	<div> <div>11%</div> <div>88%</div> <div>10%</div> <div>..</div> </div>
2	B	14	<div> <div>7%</div> <div>71%</div> <div>7%</div> <div>21%</div> </div>
2	D	14	<div> <div>14%</div> <div>57%</div> <div>7%</div> <div>7%</div> <div>29%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	9N1	A	500[A]	-	-	-	X
3	9N1	A	500[B]	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4468 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 Bile acid receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	18	0
			1977	1271	331	364	11			
1	C	230	Total	C	N	O	S	0	7	0
			1927	1236	322	357	12			

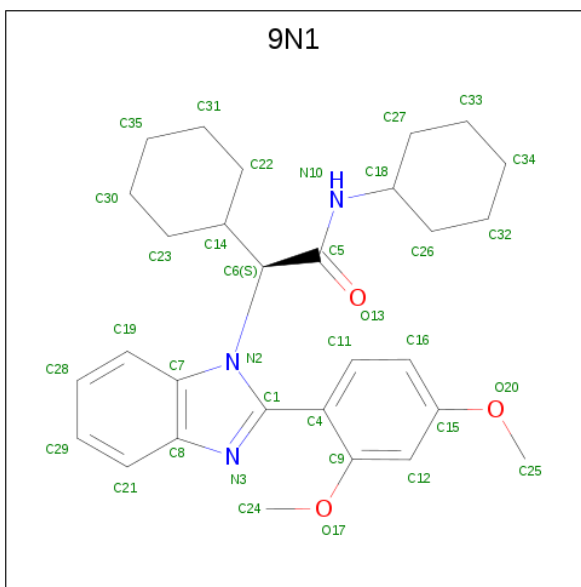
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	244	GLY	-	expression tag	UNP Q96RI1
A	245	SER	-	expression tag	UNP Q96RI1
A	246	HIS	-	expression tag	UNP Q96RI1
A	247	MET	-	expression tag	UNP Q96RI1
A	281	ALA	GLU	conflict	UNP Q96RI1
A	354	ALA	GLU	conflict	UNP Q96RI1
C	244	GLY	-	expression tag	UNP Q96RI1
C	245	SER	-	expression tag	UNP Q96RI1
C	246	HIS	-	expression tag	UNP Q96RI1
C	247	MET	-	expression tag	UNP Q96RI1
C	281	ALA	GLU	conflict	UNP Q96RI1
C	354	ALA	GLU	conflict	UNP Q96RI1

- Molecule 2 is a protein called COACTIVATOR PEPTIDE SRC-1 HD3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	11	Total	C	N	O	0	0	0
			99	64	18	17			
2	D	10	Total	C	N	O	0	0	0
			91	60	17	14			

- Molecule 3 is (2S)-N,2-dicyclohexyl-2-[2-(2,4-dimethoxyphenyl)-1H-benzimidazol-1-yl]acetamide (three-letter code: 9N1) (formula: C₂₉H₃₇N₃O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	1
			70	58	6	6		
3	C	1	Total	C	N	O	0	1
			70	58	6	6		

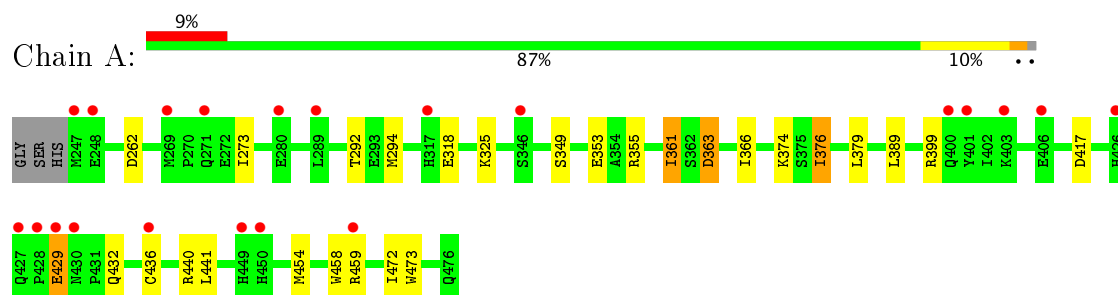
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	116	Total	O	0	0
			116	116		
4	B	6	Total	O	0	0
			6	6		
4	C	108	Total	O	0	0
			108	108		
4	D	4	Total	O	0	0
			4	4		

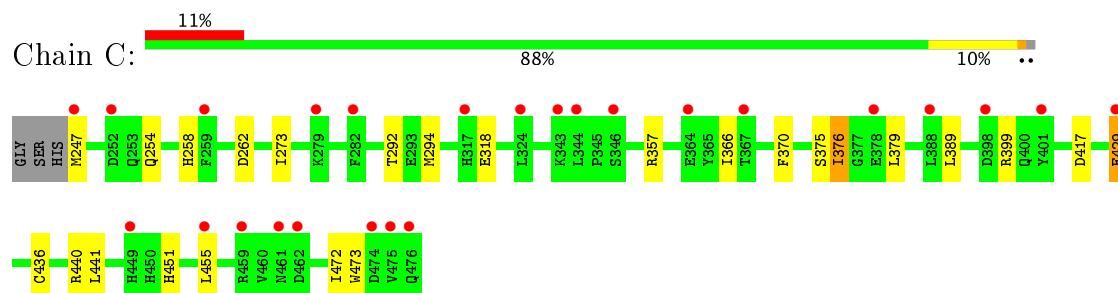
3 Residue-property plots [i](#)

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.

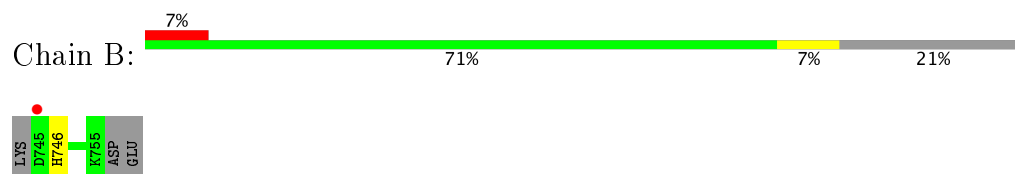
- Molecule 1: Bile acid receptor



- Molecule 1: Bile acid receptor



- Molecule 2: COACTIVATOR PEPTIDE SRC-1 HD3



- Molecule 2: COACTIVATOR PEPTIDE SRC-1 HD3



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	71.67Å 83.79Å 189.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.35 – 1.98 18.96 – 1.98	Depositor EDS
% Data completeness (in resolution range)	93.5 (19.35-1.98) 94.0 (18.96-1.98)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 1.99Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.215 , 0.237 0.226 , 0.248	Depositor DCC
R_{free} test set	1883 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	37.9	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4468	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 6.71% 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: 9N1

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	0.41	0/2073	0.57	0/2800
1	C	0.41	0/1990	0.56	0/2687
2	B	0.42	0/100	0.68	0/133
2	D	0.40	0/92	0.65	0/122
All	All	0.41	0/4255	0.57	0/5742

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1977	0	2017	11	0
1	C	1927	0	1934	11	0
2	B	99	0	101	1	0
2	D	91	0	97	1	0
3	A	70	0	0	0	0
3	C	70	0	0	0	0
4	A	116	0	0	0	0
4	B	6	0	0	0	0
4	C	108	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	4	0	0	0	0
All	All	4468	0	4149	23	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 3.

All (23) 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:273:ILE:HG12	1:A:294:MET:HE1	1.72	0.71
1:A:273:ILE:HG12	1:A:294:MET:CE	2.26	0.65
1:C:375:SER:HB2	1:C:440[B]:ARG:NH2	2.15	0.59
1:C:273:ILE:HG12	1:C:294:MET:HE1	1.84	0.59
1:C:273:ILE:HG12	1:C:294:MET:CE	2.38	0.54
1:A:379:LEU:HD21	1:A:436:CYS:HB3	1.93	0.50
1:A:363:ASP:HA	1:A:366[A]:ILE:HD12	1.94	0.49
1:C:376:ILE:HA	1:C:379:LEU:HD12	1.95	0.49
1:A:376:ILE:HA	1:A:379:LEU:HD12	1.96	0.48
1:A:472:ILE:HG22	1:A:473:TRP:CD1	2.49	0.48
1:A:429:GLU:H	1:A:429:GLU:HG2	1.50	0.46
1:C:472:ILE:HG22	1:C:473:TRP:CD1	2.50	0.45
1:A:389:LEU:HG	1:A:441:LEU:HD21	1.98	0.45
1:C:379:LEU:HD21	1:C:436:CYS:HB3	1.99	0.44
1:C:389:LEU:HG	1:C:441:LEU:HD21	2.00	0.43
1:A:349:SER:O	1:A:353[B]:GLU:HG3	2.18	0.42
1:C:451[A]:HIS:NE2	1:C:455:LEU:HD11	2.34	0.42
1:A:361[B]:ILE:HG23	1:A:458:TRP:CE3	2.54	0.42
1:A:325:LYS:HD2	2:B:746:HIS:NE2	2.35	0.42
1:C:429:GLU:H	1:C:429:GLU:HG3	1.71	0.41
1:C:357:ARG:HG3	1:C:370:PHE:CE2	2.55	0.40
2:D:749:LEU:HA	2:D:749:LEU:HD22	1.94	0.40
1:C:254:GLN:O	1:C:258:HIS:HD2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	246/233 (106%)	242 (98%)	4 (2%)	0	100	100
1	C	235/233 (101%)	231 (98%)	4 (2%)	0	100	100
2	B	9/14 (64%)	9 (100%)	0	0	100	100
2	D	8/14 (57%)	7 (88%)	1 (12%)	0	100	100
All	All	498/494 (101%)	489 (98%)	9 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	228/213 (107%)	210 (92%)	18 (8%)	14	8
1	C	218/213 (102%)	209 (96%)	9 (4%)	35	29
2	B	11/14 (79%)	11 (100%)	0	100	100
2	D	10/14 (71%)	8 (80%)	2 (20%)	1	0
All	All	467/454 (103%)	438 (94%)	29 (6%)	23	14

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	262[A]	ASP
1	A	262[B]	ASP

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Mol	Chain	Res	Type
1	A	292	THR
1	A	318	GLU
1	A	355	ARG
1	A	361[A]	ILE
1	A	361[B]	ILE
1	A	363	ASP
1	A	374	LYS
1	A	376	ILE
1	A	399	ARG
1	A	417	ASP
1	A	429	GLU
1	A	432	GLN
1	A	440	ARG
1	A	454	MET
1	A	459[A]	ARG
1	A	459[B]	ARG
1	C	247	MET
1	C	262	ASP
1	C	292	THR
1	C	318	GLU
1	C	366	ILE
1	C	376	ILE
1	C	399	ARG
1	C	417	ASP
1	C	429	GLU
2	D	749	LEU
2	D	753	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	258	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

4 ligands 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	$\# Z > 2$
3	9N1	A	500[A]	-	38,39,39	0.70	0	45,54,54	0.59	0
3	9N1	A	500[B]	-	38,39,39	0.73	0	45,54,54	0.58	0
3	9N1	C	500[A]	-	38,39,39	0.69	0	45,54,54	0.49	0
3	9N1	C	500[B]	-	38,39,39	0.72	0	45,54,54	0.63	2 (4%)

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
3	9N1	A	500[A]	-	-	0/20/40/40	0/5/5/5
3	9N1	A	500[B]	-	-	0/20/40/40	0/5/5/5
3	9N1	C	500[A]	-	-	0/20/40/40	0/5/5/5
3	9N1	C	500[B]	-	-	0/20/40/40	0/5/5/5

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	500[B]	9N1	C9-C4-C1	-2.30	119.85	122.68
3	C	500[B]	9N1	C11-C4-C1	2.01	121.85	118.69

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

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, 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	230/233 (98%)	0.66	21 (9%) 10 12	25, 45, 72, 95	0
1	C	230/233 (98%)	0.82	25 (10%) 6 7	29, 49, 75, 122	0
2	B	11/14 (78%)	1.45	1 (9%) 10 12	39, 49, 73, 98	0
2	D	10/14 (71%)	1.06	2 (20%) 1 1	44, 53, 70, 93	0
All	All	481/494 (97%)	0.76	49 (10%) 7 9	25, 48, 74, 122	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	476	GLN	9.3
1	A	247	MET	6.6
1	C	462	ASP	4.5
1	A	429	GLU	4.5
1	C	401	TYR	4.4
2	B	745	ASP	4.4
1	C	474	ASP	4.3
1	A	401	TYR	4.0
1	C	461	ASN	3.9
1	A	449	HIS	3.5
1	A	450	HIS	3.5
1	C	398	ASP	3.5
1	C	429	GLU	3.3
1	C	475	VAL	3.2
1	A	426[A]	HIS	3.1
1	C	247	MET	3.1
1	C	449	HIS	3.1
1	C	259	PHE	2.9
1	A	459[A]	ARG	2.9
1	A	346[A]	SER	2.9
1	A	428	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	388	LEU	2.6
1	C	346	SER	2.6
1	C	343	LYS	2.6
1	C	367	THR	2.6
1	A	436	CYS	2.6
1	A	400	GLN	2.5
1	C	252[A]	ASP	2.5
1	C	282	PHE	2.4
2	D	746	HIS	2.4
1	C	378	GLU	2.4
1	A	403	LYS	2.4
1	A	406[A]	GLU	2.4
1	C	344	LEU	2.4
1	C	279	LYS	2.4
1	C	317	HIS	2.3
1	A	280	GLU	2.3
1	C	324	LEU	2.3
1	A	430	ASN	2.2
1	A	269	MET	2.2
1	A	317	HIS	2.2
1	A	427[A]	GLN	2.1
1	A	248	GLU	2.1
1	C	455	LEU	2.1
2	D	754	ASP	2.1
1	A	289	LEU	2.1
1	A	271	GLN	2.0
1	C	459	ARG	2.0
1	C	364[A]	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 carbohydrates 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. 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
3	9N1	A	500[B]	35/35	0.96	0.21	2.78	30,35,40,40	35
3	9N1	A	500[A]	35/35	0.96	0.21	2.74	21,26,32,33	35
3	9N1	C	500[B]	35/35	0.96	0.21	1.91	25,30,33,33	35
3	9N1	C	500[A]	35/35	0.96	0.21	1.86	42,46,51,52	35

6.5 Other polymers

There are no such residues in this entry.