



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:52 AM UTC

PDB ID : 4NBM / pdb_00004nbm
Title : Crystal structure of UVB photoreceptor UVR8 and light-induced structural changes at 180K
Authors : Yang, X.; Zeng, X.; Zhao, K.-H.; Ren, Z.
Deposited on : 2013-10-23
Resolution : 1.61 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

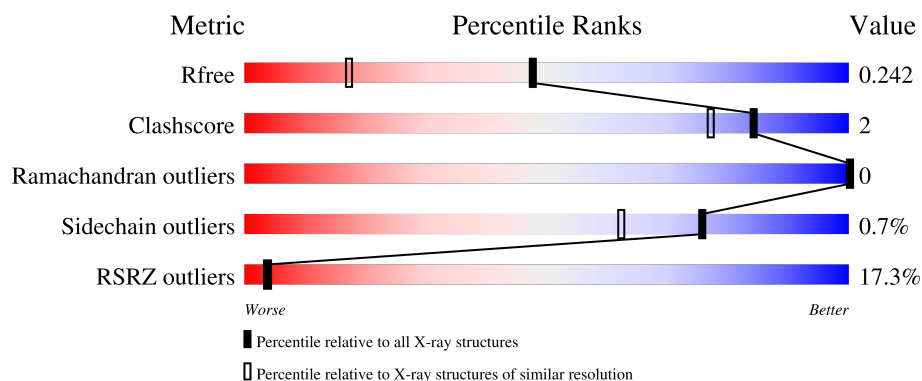
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.61 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}	180053	6728 (1.64-1.60)
Clashscore	190562	7023 (1.64-1.60)
Ramachandran outliers	187476	6898 (1.64-1.60)
Sidechain outliers	187428	6896 (1.64-1.60)
RSRZ outliers	180081	6727 (1.64-1.60)

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 $\leq 5\%$. 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	377	12% 93% 5% .
1	B	377	29% 93% 5% .
1	C	377	10% 92% 6% .
1	D	377	16% 91% 6% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13218 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 Ultraviolet-B receptor UVR8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	S	0	12	0
			2888	1797	522	553	16			
1	B	369	Total	C	N	O	S	0	10	0
			2868	1783	518	551	16			
1	C	369	Total	C	N	O	S	0	11	0
			2881	1794	523	549	15			
1	D	369	Total	C	N	O	S	0	13	0
			2892	1798	526	553	15			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	382	LEU	-	expression tag	UNP Q9FN03
A	383	GLU	-	expression tag	UNP Q9FN03
A	384	HIS	-	expression tag	UNP Q9FN03
A	385	HIS	-	expression tag	UNP Q9FN03
A	386	HIS	-	expression tag	UNP Q9FN03
A	387	HIS	-	expression tag	UNP Q9FN03
A	388	HIS	-	expression tag	UNP Q9FN03
A	389	HIS	-	expression tag	UNP Q9FN03
B	382	LEU	-	expression tag	UNP Q9FN03
B	383	GLU	-	expression tag	UNP Q9FN03
B	384	HIS	-	expression tag	UNP Q9FN03
B	385	HIS	-	expression tag	UNP Q9FN03
B	386	HIS	-	expression tag	UNP Q9FN03
B	387	HIS	-	expression tag	UNP Q9FN03
B	388	HIS	-	expression tag	UNP Q9FN03
B	389	HIS	-	expression tag	UNP Q9FN03
C	382	LEU	-	expression tag	UNP Q9FN03
C	383	GLU	-	expression tag	UNP Q9FN03
C	384	HIS	-	expression tag	UNP Q9FN03
C	385	HIS	-	expression tag	UNP Q9FN03
C	386	HIS	-	expression tag	UNP Q9FN03

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	387	HIS	-	expression tag	UNP Q9FN03
C	388	HIS	-	expression tag	UNP Q9FN03
C	389	HIS	-	expression tag	UNP Q9FN03
D	382	LEU	-	expression tag	UNP Q9FN03
D	383	GLU	-	expression tag	UNP Q9FN03
D	384	HIS	-	expression tag	UNP Q9FN03
D	385	HIS	-	expression tag	UNP Q9FN03
D	386	HIS	-	expression tag	UNP Q9FN03
D	387	HIS	-	expression tag	UNP Q9FN03
D	388	HIS	-	expression tag	UNP Q9FN03
D	389	HIS	-	expression tag	UNP Q9FN03

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	7	Total 7	Mg 7	0	0
2	B	3	Total 3	Mg 3	0	0
2	C	8	Total 8	Mg 8	0	0
2	D	5	Total 5	Mg 5	0	0

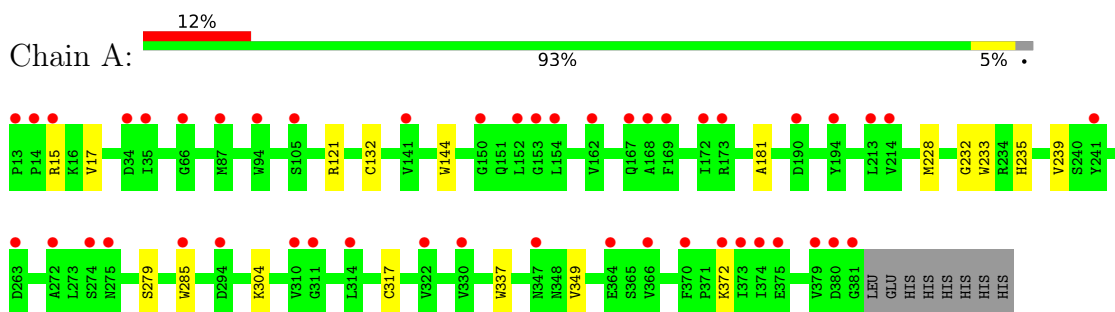
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	440	Total 440	O 440	0	0
3	B	399	Total 399	O 399	0	0
3	C	418	Total 418	O 418	0	0
3	D	409	Total 409	O 409	0	0

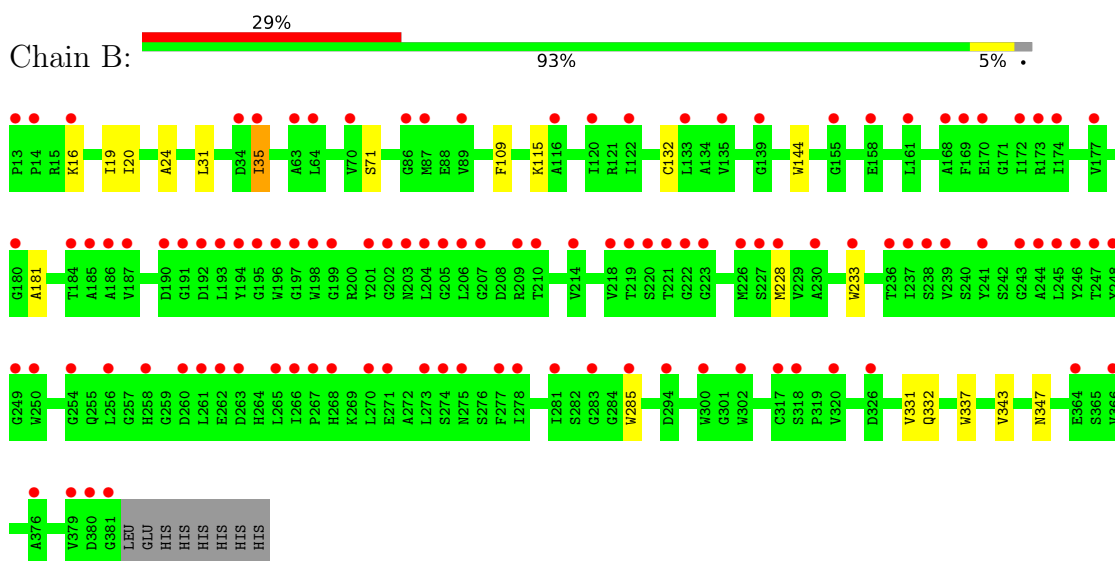
3 Residue-property plots [i](#)

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.

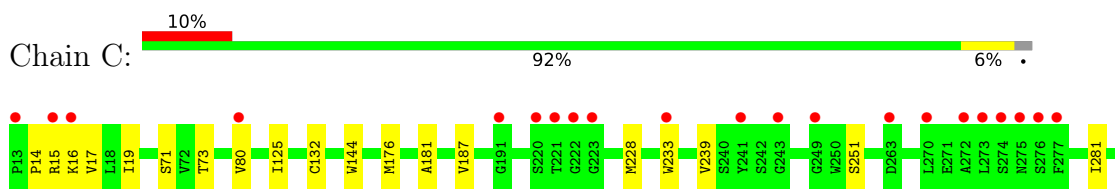
• Molecule 1: Ultraviolet-B receptor UVR8

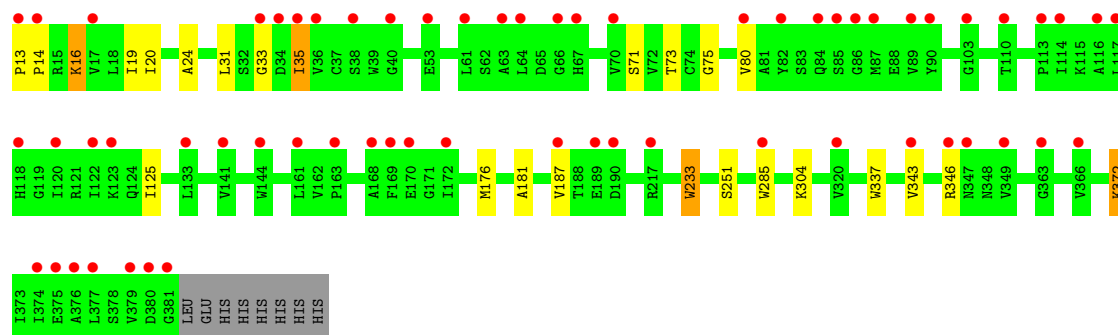


• Molecule 1: Ultraviolet-B receptor UVR8



• Molecule 1: Ultraviolet-B receptor UVR8





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	113.31Å 76.83Å 191.25Å 90.00° 96.75° 90.00°	Depositor
Resolution (Å)	29.86 – 1.61 29.86 – 1.61	Depositor EDS
% Data completeness (in resolution range)	78.5 (29.86-1.61) 72.3 (29.86-1.61)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 1.79Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.150 , 0.182 0.226 , 0.242	Depositor DCC
R_{free} test set	5473 reflections (2.55%)	wwPDB-VP
Wilson B-factor (Å ²)	14.1	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13218	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.15 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0344e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: MG

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	0.42	0/2962	0.70	0/4014
1	B	0.40	0/2939	0.70	0/3985
1	C	0.40	0/2955	0.71	0/4006
1	D	0.39	0/2966	0.68	2/4020 (0.0%)
All	All	0.40	0/11822	0.70	2/16025 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	33	GLY	N-CA-C	-5.33	107.91	115.43
1	D	75	GLY	N-CA-C	-5.03	105.68	112.57

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	2888	0	2760	12	0
1	B	2868	0	2736	13	0
1	C	2881	0	2760	14	0
1	D	2892	0	2766	14	0
2	A	7	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3	0	0	0	0
2	C	8	0	0	0	0
2	D	5	0	0	0	0
3	A	440	0	0	4	0
3	B	399	0	0	2	0
3	C	418	0	0	3	0
3	D	409	0	0	2	0
All	All	13218	0	11022	52	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 2.

All (52) 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:228[A]:MET:HE3	1:A:239:VAL:HG21	1.76	0.67
1:D:304:LYS:NZ	3:D:875:HOH:O	2.29	0.65
1:A:317[A]:CYS:SG	3:A:744:HOH:O	2.55	0.64
1:A:317[B]:CYS:SG	3:A:744:HOH:O	2.56	0.61
1:B:115:LYS:NZ	3:B:767:HOH:O	2.23	0.58
1:A:285:TRP:HB2	1:A:337:TRP:HA	1.85	0.58
1:C:80[B]:VAL:HG11	1:C:125:ILE:HG21	1.86	0.57
1:C:285:TRP:HB2	1:C:337:TRP:HA	1.86	0.57
1:C:14:PRO:HB2	1:C:16:LYS:HE3	1.86	0.57
1:D:181:ALA:HB2	1:D:233:TRP:CD1	2.40	0.56
1:B:19:ILE:HD12	1:B:71:SER:HA	1.87	0.56
1:C:17:VAL:HG21	1:C:349:VAL:HG21	1.87	0.56
1:B:285:TRP:HB2	1:B:337:TRP:HA	1.88	0.55
1:D:285:TRP:HB2	1:D:337:TRP:HA	1.87	0.55
1:A:15:ARG:NE	3:A:777:HOH:O	2.38	0.55
1:A:17:VAL:HG21	1:A:349:VAL:HG21	1.90	0.54
1:A:228[A]:MET:HE1	1:A:279[A]:SER:C	2.32	0.53
1:D:80[B]:VAL:HG11	1:D:125:ILE:HG21	1.90	0.53
1:C:15:ARG:NE	3:C:754:HOH:O	2.29	0.51
1:C:372:LYS:HG2	3:C:747:HOH:O	2.09	0.51
1:B:20:ILE:HD13	1:B:343:VAL:HG23	1.92	0.51
1:D:20:ILE:HD13	1:D:343:VAL:HG23	1.94	0.50
1:D:19:ILE:HD12	1:D:71:SER:HA	1.93	0.50
1:C:228:MET:HE3	1:C:281:ILE:HG12	1.95	0.49
1:C:132:CYS:HB2	1:C:144:TRP:CE2	2.49	0.48
1:B:16:LYS:HA	1:B:347:ASN:HD21	1.78	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:LYS:HE2	1:B:109:PHE:CZ	2.50	0.47
1:B:331:VAL:HG23	1:B:332:GLN:HG3	1.97	0.46
1:D:346[A]:ARG:NE	3:D:800:HOH:O	2.47	0.45
1:D:13:PRO:HA	1:D:14:PRO:HD3	1.87	0.45
1:C:19:ILE:HD12	1:C:71:SER:HA	1.98	0.45
1:D:31:LEU:HD12	1:D:35:ILE:HD11	1.98	0.45
1:C:228:MET:HE2	1:C:239:VAL:HG21	1.97	0.45
1:B:181:ALA:HB2	1:B:233:TRP:CD1	2.52	0.44
1:C:73:THR:HB	1:C:80[B]:VAL:HG12	2.00	0.44
1:C:181:ALA:HB2	1:C:233:TRP:CD1	2.53	0.43
1:C:329:LYS:NZ	3:C:511:HOH:O	2.50	0.43
1:D:372:LYS:HE3	1:D:372:LYS:HB3	1.83	0.43
1:A:181:ALA:HB2	1:A:233:TRP:CD1	2.54	0.43
1:D:176:MET:HG2	1:D:187:VAL:HG22	2.00	0.43
1:A:232:GLY:HA3	1:A:235:HIS:CE1	2.54	0.42
1:D:73:THR:HB	1:D:80[B]:VAL:HG12	1.99	0.42
1:D:24:ALA:HA	1:D:337:TRP:CD1	2.55	0.42
1:B:228:MET:HE2	3:B:601:HOH:O	2.19	0.41
1:B:31:LEU:HD12	1:B:35:ILE:HD11	2.02	0.41
1:B:24:ALA:HA	1:B:337:TRP:CD1	2.55	0.41
1:D:16:LYS:HE2	1:D:16:LYS:HB3	1.89	0.41
1:A:121[B]:ARG:HD2	3:A:715:HOH:O	2.21	0.41
1:C:176:MET:HG2	1:C:187:VAL:HG22	2.03	0.41
1:B:132:CYS:HB2	1:B:144:TRP:CE2	2.56	0.40
1:A:132:CYS:HB2	1:A:144:TRP:CE2	2.57	0.40
1:B:16:LYS:HA	1:B:347:ASN:ND2	2.36	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	379/377 (100%)	377 (100%)	2 (0%)	0	100	100
1	B	377/377 (100%)	376 (100%)	1 (0%)	0	100	100
1	C	378/377 (100%)	376 (100%)	2 (0%)	0	100	100
1	D	380/377 (101%)	377 (99%)	3 (1%)	0	100	100
All	All	1514/1508 (100%)	1506 (100%)	8 (0%)	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	304/300 (101%)	303 (100%)	1 (0%)	86	79
1	B	302/300 (101%)	301 (100%)	1 (0%)	86	79
1	C	303/300 (101%)	302 (100%)	1 (0%)	86	79
1	D	305/300 (102%)	300 (98%)	5 (2%)	55	32
All	All	1214/1200 (101%)	1206 (99%)	8 (1%)	76	62

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	372	LYS
1	B	35	ILE
1	C	251	SER
1	D	16	LYS
1	D	35	ILE
1	D	233	TRP
1	D	251	SER
1	D	372	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	ASN
1	A	203	ASN
1	A	357	ASN
1	B	167	GLN
1	B	203	ASN
1	B	357	ASN
1	C	149	ASN
1	C	203	ASN
1	C	347	ASN
1	D	149	ASN
1	D	203	ASN
1	D	357	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 23 are 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 ⓘ

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	369/377 (97%)	1.13	47 (12%) 8 8	10, 19, 39, 76	12 (3%)
1	B	369/377 (97%)	1.57	110 (29%) 1 1	9, 22, 40, 76	10 (2%)
1	C	369/377 (97%)	1.05	36 (9%) 13 13	9, 20, 39, 80	11 (2%)
1	D	369/377 (97%)	1.20	62 (16%) 4 4	10, 23, 39, 86	13 (3%)
All	All	1476/1508 (97%)	1.24	255 (17%) 4 4	9, 21, 40, 86	46 (3%)

All (255) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	13	PRO	6.0
1	B	13	PRO	5.0
1	C	13	PRO	5.0
1	A	379	VAL	4.9
1	D	381	GLY	4.8
1	B	202	GLY	4.8
1	A	13	PRO	4.6
1	D	14	PRO	4.6
1	A	381	GLY	4.6
1	B	207	GLY	4.3
1	A	87[A]	MET	4.1
1	C	380	ASP	4.1
1	B	246	TYR	4.1
1	C	381	GLY	4.0
1	B	244	ALA	3.9
1	B	219	THR	3.8
1	C	221	THR	3.8
1	B	223	GLY	3.8
1	A	380	ASP	3.8
1	B	187	VAL	3.7
1	C	379	VAL	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	14	PRO	3.7
1	D	380	ASP	3.7
1	C	275[A]	ASN	3.7
1	B	87[A]	MET	3.6
1	B	366	VAL	3.6
1	B	250	TRP	3.6
1	B	218	VAL	3.6
1	B	381	GLY	3.5
1	B	273	LEU	3.5
1	C	285	TRP	3.5
1	B	379	VAL	3.5
1	B	221	THR	3.5
1	C	241	TYR	3.4
1	D	80[A]	VAL	3.4
1	D	379	VAL	3.4
1	B	193	LEU	3.3
1	C	220	SER	3.3
1	D	376	ALA	3.3
1	A	14	PRO	3.3
1	B	214	VAL	3.3
1	C	15	ARG	3.3
1	B	196	TRP	3.2
1	B	275	ASN	3.2
1	B	155	GLY	3.2
1	B	227	SER	3.2
1	A	15	ARG	3.2
1	B	249	GLY	3.2
1	A	172	ILE	3.1
1	B	120	ILE	3.1
1	C	294	ASP	3.1
1	B	285	TRP	3.1
1	C	331	VAL	3.1
1	B	318[A]	SER	3.1
1	B	248	TYR	3.1
1	B	204	LEU	3.1
1	B	186	ALA	3.0
1	B	236	THR	3.0
1	D	33	GLY	3.0
1	A	366	VAL	3.0
1	B	194	TYR	3.0
1	D	34	ASP	3.0
1	B	158	GLU	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	233	TRP	2.9
1	B	256	LEU	2.9
1	B	278	ILE	2.9
1	B	201	TYR	2.9
1	B	195	GLY	2.9
1	A	162	VAL	2.9
1	B	230	ALA	2.9
1	C	276	SER	2.9
1	A	169	PHE	2.8
1	D	36	VAL	2.8
1	C	222	GLY	2.8
1	D	85	SER	2.8
1	B	274	SER	2.8
1	B	380	ASP	2.8
1	B	243	GLY	2.8
1	A	168	ALA	2.8
1	A	347	ASN	2.8
1	A	154	LEU	2.8
1	D	64	LEU	2.8
1	B	190	ASP	2.8
1	B	197	GLY	2.8
1	C	16	LYS	2.7
1	B	265	LEU	2.7
1	A	190[A]	ASP	2.7
1	B	210	THR	2.7
1	B	267	PRO	2.7
1	C	263	ASP	2.7
1	B	89	VAL	2.7
1	B	199	GLY	2.7
1	B	169	PHE	2.7
1	A	375	GLU	2.7
1	B	364[A]	GLU	2.7
1	D	170	GLU	2.7
1	B	320	VAL	2.7
1	A	66	GLY	2.7
1	C	223	GLY	2.7
1	C	272	ALA	2.7
1	A	370	PHE	2.6
1	B	277	PHE	2.6
1	B	205	GLY	2.6
1	B	270	LEU	2.6
1	D	90	TYR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	300	TRP	2.6
1	D	35	ILE	2.6
1	A	34	ASP	2.6
1	D	168	ALA	2.6
1	B	226	MET	2.6
1	B	139	GLY	2.6
1	B	173	ARG	2.6
1	C	80[A]	VAL	2.6
1	B	222	GLY	2.6
1	B	133	LEU	2.6
1	B	206	LEU	2.6
1	C	317[A]	CYS	2.6
1	D	141	VAL	2.6
1	D	122	ILE	2.6
1	B	203	ASN	2.6
1	A	311	GLY	2.5
1	B	220	SER	2.5
1	C	274	SER	2.5
1	D	346[A]	ARG	2.5
1	A	373	ILE	2.5
1	B	260	ASP	2.5
1	A	150	GLY	2.5
1	D	116	ALA	2.5
1	A	153	GLY	2.5
1	C	318	SER	2.5
1	C	277	PHE	2.5
1	B	63	ALA	2.5
1	B	239	VAL	2.5
1	D	118	HIS	2.5
1	D	172	ILE	2.5
1	D	285	TRP	2.4
1	B	261	LEU	2.4
1	D	169	PHE	2.4
1	B	283	GLY	2.4
1	D	66	GLY	2.4
1	B	241	TYR	2.4
1	A	105	SER	2.4
1	B	174	ILE	2.4
1	D	17	VAL	2.4
1	A	294	ASP	2.4
1	B	34	ASP	2.4
1	A	364	GLU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	16	LYS	2.4
1	B	209[A]	ARG	2.4
1	A	214	VAL	2.4
1	A	263	ASP	2.4
1	B	262	GLU	2.4
1	A	173[A]	ARG	2.4
1	D	123	LYS	2.4
1	B	191	GLY	2.4
1	D	84	GLN	2.4
1	A	213	LEU	2.4
1	B	245	LEU	2.4
1	D	161	LEU	2.4
1	D	63	ALA	2.4
1	A	241	TYR	2.4
1	B	122	ILE	2.4
1	B	237	ILE	2.4
1	B	228	MET	2.4
1	D	87	MET	2.4
1	C	243	GLY	2.3
1	C	284	GLY	2.3
1	B	317[A]	CYS	2.3
1	A	194	TYR	2.3
1	D	82	TYR	2.3
1	A	167	GLN	2.3
1	A	310	VAL	2.3
1	D	89	VAL	2.3
1	D	189	GLU	2.3
1	B	161	LEU	2.3
1	C	273	LEU	2.3
1	D	67	HIS	2.3
1	B	35	ILE	2.3
1	B	170	GLU	2.3
1	A	285	TRP	2.3
1	D	86	GLY	2.3
1	D	190	ASP	2.3
1	B	247	THR	2.3
1	B	168	ALA	2.3
1	B	185	ALA	2.3
1	A	314	LEU	2.3
1	D	61	LEU	2.3
1	D	377	LEU	2.3
1	C	233	TRP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	238	SER	2.2
1	B	263	ASP	2.2
1	C	327	ASP	2.2
1	A	374	ILE	2.2
1	D	114	ILE	2.2
1	D	374	ILE	2.2
1	D	70	VAL	2.2
1	D	217[A]	ARG	2.2
1	D	347	ASN	2.2
1	C	355	GLY	2.2
1	D	40	GLY	2.2
1	B	271	GLU	2.2
1	C	372	LYS	2.2
1	D	38	SER	2.2
1	B	376	ALA	2.2
1	A	94	TRP	2.2
1	B	198	TRP	2.2
1	D	375	GLU	2.2
1	B	266	ILE	2.2
1	C	320	VAL	2.1
1	C	249	GLY	2.1
1	B	302	TRP	2.1
1	C	270	LEU	2.1
1	B	184	THR	2.1
1	D	113	PRO	2.1
1	D	163	PRO	2.1
1	A	141	VAL	2.1
1	A	322	VAL	2.1
1	B	70	VAL	2.1
1	B	116	ALA	2.1
1	D	187	VAL	2.1
1	C	191	GLY	2.1
1	D	103	GLY	2.1
1	B	64	LEU	2.1
1	D	144	TRP	2.1
1	C	305	PHE	2.1
1	A	330	VAL	2.1
1	D	320[A]	VAL	2.1
1	D	343	VAL	2.1
1	D	53[A]	GLU	2.1
1	B	192	ASP	2.1
1	B	294	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	110	THR	2.1
1	A	35	ILE	2.1
1	B	180	GLY	2.0
1	B	254	GLY	2.0
1	D	363	GLY	2.0
1	A	272	ALA	2.0
1	A	274	SER	2.0
1	B	135	VAL	2.0
1	B	326	ASP	2.0
1	D	366	VAL	2.0
1	A	152	LEU	2.0
1	D	117	LEU	2.0
1	D	133	LEU	2.0
1	B	258	HIS	2.0
1	B	268	HIS	2.0
1	A	275	ASN	2.0
1	B	86	GLY	2.0
1	B	172	ILE	2.0
1	B	281	ILE	2.0
1	D	120	ILE	2.0
1	B	177	VAL	2.0
1	C	322	VAL	2.0
1	D	349	VAL	2.0
1	A	372	LYS	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	MG	C	402	1/1	0.59	0.22	48,48,48,48	0
2	MG	D	402	1/1	0.69	0.17	54,54,54,54	0
2	MG	B	401	1/1	0.70	0.17	64,64,64,64	0
2	MG	D	401	1/1	0.76	0.15	42,42,42,42	0
2	MG	D	403	1/1	0.77	0.11	53,53,53,53	0
2	MG	A	406	1/1	0.78	0.13	51,51,51,51	0
2	MG	C	408	1/1	0.80	0.21	41,41,41,41	0
2	MG	B	402	1/1	0.80	0.13	57,57,57,57	0
2	MG	D	404	1/1	0.83	0.12	44,44,44,44	0
2	MG	A	404	1/1	0.84	0.24	39,39,39,39	0
2	MG	A	403	1/1	0.85	0.12	34,34,34,34	0
2	MG	C	403	1/1	0.86	0.08	47,47,47,47	0
2	MG	A	401	1/1	0.87	0.11	37,37,37,37	0
2	MG	C	407	1/1	0.88	0.11	54,54,54,54	0
2	MG	C	404	1/1	0.88	0.19	46,46,46,46	0
2	MG	D	405	1/1	0.90	0.18	48,48,48,48	0
2	MG	C	405	1/1	0.91	0.11	41,41,41,41	0
2	MG	A	405	1/1	0.91	0.12	34,34,34,34	0
2	MG	C	401	1/1	0.92	0.09	31,31,31,31	0
2	MG	A	402	1/1	0.92	0.09	32,32,32,32	0
2	MG	B	403	1/1	0.93	0.07	59,59,59,59	0
2	MG	A	407	1/1	0.96	0.06	19,19,19,19	0
2	MG	C	406	1/1	0.97	0.08	20,20,20,20	0

6.5 Other polymers

There are no such residues in this entry.