



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:56 AM UTC

PDB ID : 6XLZ / pdb_00006xlz
Title : Structure of NHP D11A.F2 Fab in complex with 16055 V2b peptide
Authors : Aljedani, S.; Rodarte, J.; Liban, T.; Pancera, M.
Deposited on : 2020-06-29
Resolution : 2.80 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

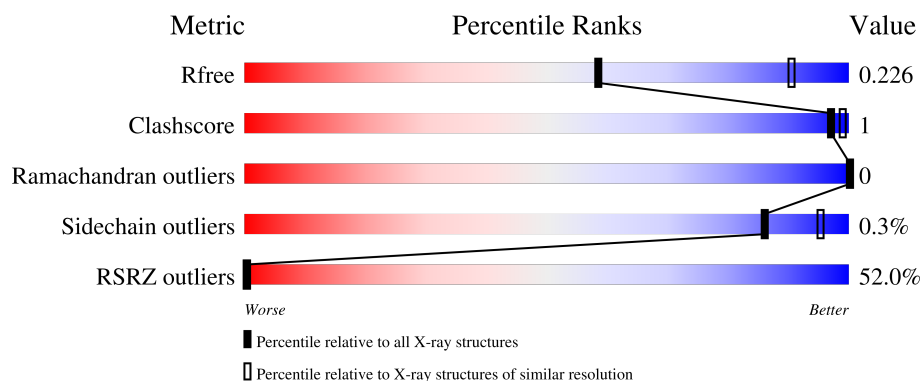
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	23	26% 26% 74%
1	P	23	26% 74% 9% 13%
2	H	222	60% 93% . .
3	L	217	42% 96% . .

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BU3	H	303	-	-	-	X
5	SO4	H	304	-	-	-	X
5	SO4	L	304	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7160 atoms, of which 3555 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 Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	20	Total	C	H	N	O	0	0	0
			317	101	155	29	32			
1	A	6	Total	C	H	N	O	0	0	0
			116	36	62	10	8			

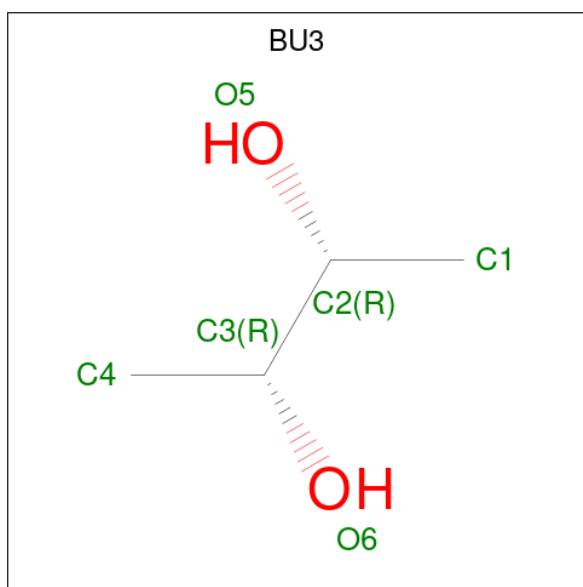
- Molecule 2 is a protein called NHP_D11A.F2_Fab_Heavy_chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	214	Total	C	H	N	O	S	0	0	0
			3161	1012	1561	269	313	6			

- Molecule 3 is a protein called NHP_D11A.F2_Fab_Light_Chain.

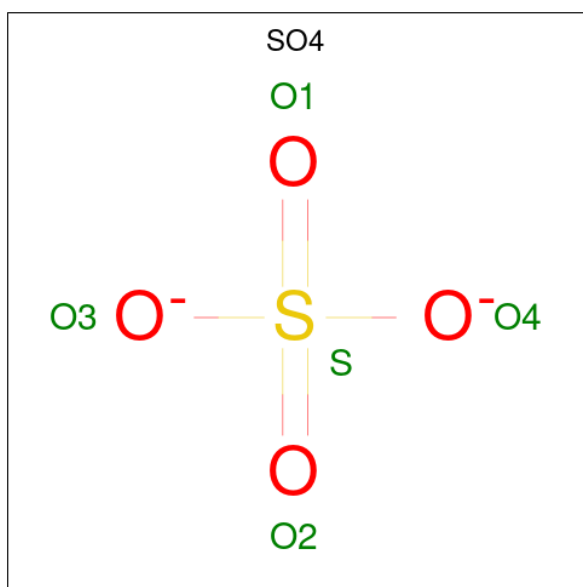
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	L	214	Total	C	H	N	O	S	0	0	0
			3126	1000	1515	271	336	4			

- Molecule 4 is (R,R)-2,3-BUTANEDIOL (CCD ID: BU3) (formula: C₄H₁₀O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	H	O	0	0
			16	4	10	2		
4	H	1	Total	C	H	O	0	0
			16	4	10	2		
4	H	1	Total	C	H	O	0	0
			16	4	10	2		
4	H	1	Total	C	H	O	0	0
			16	4	10	2		
4	L	1	Total	C	H	O	0	0
			16	4	10	2		
4	L	1	Total	C	H	O	0	0
			16	4	10	2		
4	L	1	Total	C	H	O	0	0
			16	4	10	2		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	H	1	Total	O	S	0	0
			5	4	1		
5	H	1	Total	O	S	0	0
			5	4	1		
5	H	1	Total	O	S	0	0
			5	4	1		
5	H	1	Total	O	S	0	0
			5	4	1		
5	H	1	Total	O	S	0	0
			5	4	1		
5	L	1	Total	O	S	0	0
			5	4	1		
5	L	1	Total	O	S	0	0
			5	4	1		
5	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	P	10	Total	H	O	0	0
			30	20	10		
6	H	39	Total	H	O	0	0
			117	78	39		
6	L	47	Total	H	O	0	0
			141	94	47		

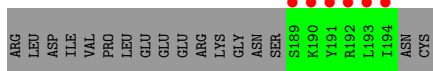
3 Residue-property plots [i](#)

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.

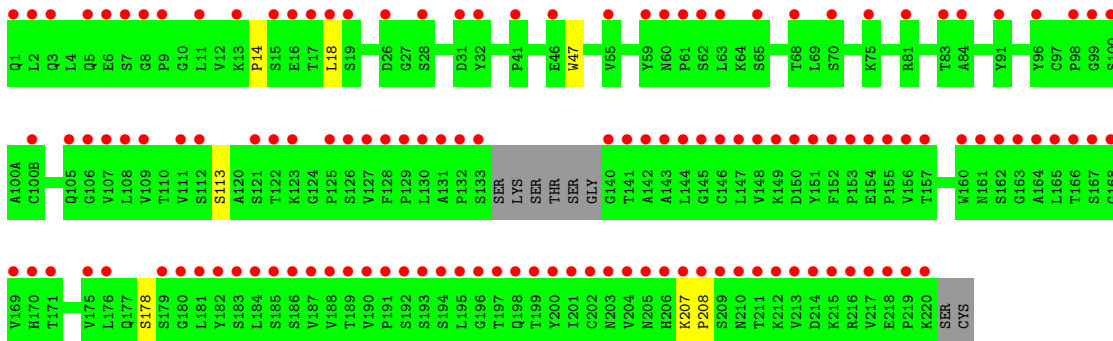
- Molecule 1: Envelope glycoprotein gp160



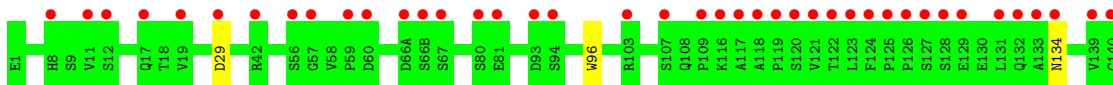
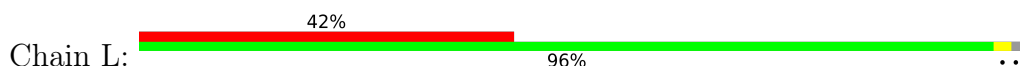
- Molecule 1: Envelope glycoprotein gp160

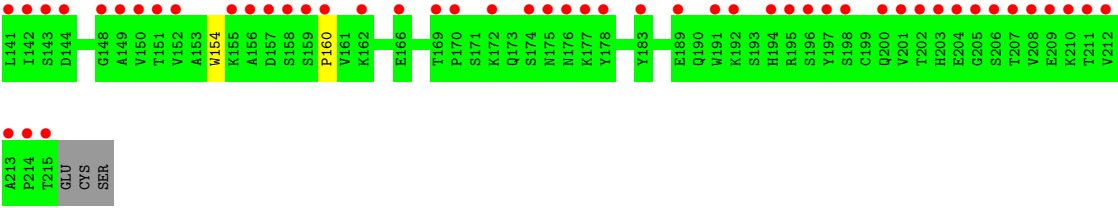


- Molecule 2: NHP_D11A.F2_Fab_Heavy_chain



- Molecule 3: NHP_D11A.F2_Fab_Light_Chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	130.39Å 130.39Å 170.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	94.21 – 2.80 94.21 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (94.21-2.80) 99.7 (94.21-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.82Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.216 , 0.255 (Not available) , 0.226	Depositor DCC
R_{free} test set	1092 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	38.9	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 67.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	7160	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% 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: BU3, SO4

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	0/54	0.59	0/70
1	P	1.74	4/163 (2.5%)	1.19	2/217 (0.9%)
2	H	0.28	0/1641	0.52	0/2251
3	L	0.51	2/1651 (0.1%)	0.55	0/2258
All	All	0.55	6/3509 (0.2%)	0.58	2/4796 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	182	VAL	C-N	12.83	1.50	1.33
1	P	181	ILE	C-O	-11.29	1.11	1.24
1	P	182	VAL	C-O	-8.74	1.13	1.24
3	L	160	PRO	C-O	-8.58	1.14	1.23
3	L	154	TRP	C-O	-6.39	1.15	1.24
1	P	180	ASP	C-O	-5.85	1.16	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	182	VAL	CA-C-N	7.68	128.28	119.99
1	P	182	VAL	C-N-CA	7.68	128.28	119.99

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	54	62	61	0	0
1	P	162	155	163	1	1
2	H	1600	1561	1561	4	1
3	L	1611	1515	1524	3	1
4	H	24	40	40	0	0
4	L	18	30	30	0	0
5	H	25	0	0	0	0
5	L	15	0	0	0	0
6	H	39	78	0	0	0
6	L	47	94	0	1	0
6	P	10	20	0	0	0
All	All	3605	3555	3379	6	2

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 (6) 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)
3:L:29:ASP:OD2	6:L:401:HOH:O	1.96	0.83
2:H:47:TRP:CG	3:L:96:TRP:HB2	2.47	0.49
2:H:207:LYS:N	2:H:208:PRO:CD	2.82	0.43
2:H:14:PRO:HD2	2:H:113:SER:HB3	2.01	0.41
2:H:47:TRP:CD1	3:L:96:TRP:HB2	2.55	0.41
1:P:182:VAL:O	1:P:182:VAL:HG23	2.20	0.41

All (2) 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)
1:P:181:ILE:CD1	1:P:181:ILE:CD1[9_554]	1.64	0.56
2:H:178:SER:OG	3:L:134:ASN:OD1[12_565]	2.14	0.06

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	4/23 (17%)	4 (100%)	0	0	100	100
1	P	18/23 (78%)	18 (100%)	0	0	100	100
2	H	210/222 (95%)	204 (97%)	6 (3%)	0	100	100
3	L	212/217 (98%)	208 (98%)	4 (2%)	0	100	100
All	All	444/485 (92%)	434 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	6/22 (27%)	6 (100%)	0	100	100
1	P	18/22 (82%)	18 (100%)	0	100	100
2	H	183/194 (94%)	182 (100%)	1 (0%)	81	93
3	L	183/188 (97%)	183 (100%)	0	100	100
All	All	390/426 (92%)	389 (100%)	1 (0%)	86	95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	18	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such

sidechains are listed below:

Mol	Chain	Res	Type
2	H	76	ASN
2	H	161	ASN
3	L	17	GLN
3	L	53	GLN
3	L	108	GLN
3	L	194	HIS

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](#)

15 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	$\# Z > 2$
5	SO4	H	304	-	4,4,4	0.24	0	6,6,6	0.08	0
5	SO4	L	303	-	4,4,4	0.23	0	6,6,6	0.07	0
4	BU3	H	302	-	4,5,5	0.75	0	6,6,6	0.45	0
4	BU3	L	301	-	4,5,5	0.87	0	6,6,6	0.42	0
4	BU3	H	303	-	4,5,5	0.92	0	6,6,6	0.50	0
5	SO4	L	302	-	4,4,4	0.21	0	6,6,6	0.08	0
5	SO4	H	307	-	4,4,4	0.23	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BU3	L	305	-	4,5,5	0.83	0	6,6,6	0.52	0
4	BU3	L	306	-	4,5,5	0.75	0	6,6,6	0.46	0
4	BU3	H	301	-	4,5,5	0.78	0	6,6,6	0.44	0
5	SO4	H	305	-	4,4,4	0.23	0	6,6,6	0.09	0
5	SO4	H	306	-	4,4,4	0.22	0	6,6,6	0.09	0
4	BU3	H	309	-	4,5,5	0.78	0	6,6,6	0.42	0
5	SO4	H	308	-	4,4,4	0.24	0	6,6,6	0.08	0
5	SO4	L	304	-	4,4,4	0.23	0	6,6,6	0.11	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
4	BU3	H	302	-	-	0/4/4/4	-
4	BU3	L	301	-	-	0/4/4/4	-
4	BU3	H	303	-	-	4/4/4/4	-
4	BU3	L	305	-	-	0/4/4/4	-
4	BU3	L	306	-	-	0/4/4/4	-
4	BU3	H	301	-	-	0/4/4/4	-
4	BU3	H	309	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	303	BU3	C1-C2-C3-O6
4	H	303	BU3	O5-C2-C3-C4
4	H	303	BU3	C1-C2-C3-C4
4	H	303	BU3	O5-C2-C3-O6

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	6/23 (26%)	3.39	6 (100%) 0 0	63, 70, 89, 92	0
1	P	20/23 (86%)	1.94	6 (30%) 1 1	42, 50, 73, 80	0
2	H	214/222 (96%)	2.61	133 (62%) 0 0	34, 65, 109, 134	0
3	L	214/217 (98%)	2.02	91 (42%) 0 0	29, 58, 89, 100	0
All	All	454/485 (93%)	2.31	236 (51%) 0 0	29, 61, 103, 134	0

All (236) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	199	THR	8.5
2	H	195	LEU	8.1
2	H	133	SER	6.6
2	H	189	THR	6.5
2	H	197	THR	6.4
2	H	142	ALA	6.4
1	A	189	SER	5.9
2	H	200	TYR	5.9
2	H	218	GLU	5.4
2	H	140	GLY	5.4
2	H	190	VAL	5.4
3	L	124	PHE	5.3
1	P	179	LEU	5.3
2	H	202	CYS	5.3
3	L	122	THR	5.2
2	H	214	ASP	5.2
2	H	168	GLY	5.2
2	H	141	THR	5.1
2	H	131	ALA	5.0
2	H	219	PRO	4.9
2	H	55	VAL	4.9

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Mol	Chain	Res	Type	RSRZ
2	H	1	GLN	4.7
2	H	198	GLN	4.6
3	L	204	GLU	4.6
2	H	194	SER	4.6
2	H	144	LEU	4.6
3	L	120	SER	4.6
2	H	220	LYS	4.5
2	H	166	THR	4.4
2	H	143	ALA	4.4
3	L	215	THR	4.4
2	H	157	THR	4.4
2	H	187	VAL	4.3
2	H	205	ASN	4.3
1	P	194	ILE	4.2
2	H	192	SER	4.2
2	H	170	HIS	4.2
2	H	160	TRP	4.2
2	H	201	ILE	4.2
3	L	123	LEU	4.2
2	H	65	SER	4.1
3	L	205	GLY	4.1
2	H	132	PRO	4.1
2	H	167	SER	4.1
2	H	216	ARG	4.0
2	H	165	LEU	4.0
2	H	213	VAL	4.0
2	H	41	PRO	3.9
2	H	146	CYS	3.9
3	L	156	ALA	3.9
2	H	210	ASN	3.9
2	H	182	TYR	3.9
3	L	192	LYS	3.9
3	L	128	SER	3.9
3	L	196	SER	3.9
3	L	157	ASP	3.8
2	H	129	PRO	3.8
2	H	15	SER	3.7
3	L	116	LYS	3.7
3	L	197	TYR	3.7
2	H	188	VAL	3.7
2	H	212	LYS	3.7
3	L	158	SER	3.7

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Mol	Chain	Res	Type	RSRZ
2	H	208	PRO	3.6
2	H	19	SER	3.6
3	L	17	GLN	3.6
2	H	81	ARG	3.6
3	L	129	GLU	3.5
1	A	190	LYS	3.5
2	H	191	PRO	3.5
3	L	195	ARG	3.5
3	L	132	GLN	3.5
3	L	209	GLU	3.5
2	H	162	SER	3.5
3	L	107	SER	3.5
2	H	18	LEU	3.5
2	H	164	ALA	3.5
3	L	198	SER	3.4
3	L	60	ASP	3.4
2	H	196	GLY	3.4
3	L	206	SER	3.4
3	L	118	ALA	3.4
2	H	204	VAL	3.4
2	H	183	SER	3.4
3	L	149	ALA	3.4
3	L	210	LYS	3.4
1	P	181	ILE	3.3
3	L	119	PRO	3.3
3	L	194	HIS	3.3
2	H	100	SER	3.3
3	L	144	ASP	3.3
3	L	80	SER	3.3
2	H	151	TYR	3.3
3	L	117	ALA	3.3
3	L	121	VAL	3.3
3	L	155	LYS	3.2
3	L	131	LEU	3.2
2	H	105	GLN	3.2
3	L	143	SER	3.2
2	H	181	LEU	3.2
3	L	200	GLN	3.2
3	L	151	THR	3.2
3	L	176	ASN	3.2
2	H	5	GLN	3.2
2	H	207	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
3	L	208	VAL	3.2
2	H	16	GLU	3.1
3	L	81	GLU	3.1
2	H	7	SER	3.1
3	L	212	VAL	3.1
2	H	186	SER	3.1
1	P	192	ARG	3.1
2	H	184	LEU	3.1
2	H	169	VAL	3.0
2	H	193	SER	3.0
2	H	3	GLN	3.0
2	H	100(B)	CYS	3.0
2	H	8	GLY	3.0
2	H	156	VAL	3.0
3	L	178	TYR	3.0
2	H	161	ASN	3.0
2	H	153	PRO	3.0
2	H	31	ASP	2.9
3	L	207	THR	2.9
3	L	141	LEU	2.9
1	A	191	TYR	2.9
2	H	211	THR	2.9
2	H	9	PRO	2.9
3	L	162	LYS	2.9
3	L	211	THR	2.9
2	H	13	LYS	2.8
2	H	99	GLY	2.8
3	L	214	PRO	2.8
1	P	187	ASN	2.8
2	H	130	LEU	2.8
3	L	169	THR	2.8
1	A	193	LEU	2.8
2	H	68	THR	2.8
2	H	112	SER	2.8
2	H	163	GLY	2.8
2	H	155	PRO	2.8
2	H	2	LEU	2.8
2	H	121	SER	2.8
3	L	148	GLY	2.8
2	H	111	VAL	2.7
3	L	12	SER	2.7
3	L	159	SER	2.7

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Mol	Chain	Res	Type	RSRZ
3	L	19	VAL	2.7
1	A	194	ILE	2.7
3	L	175	ASN	2.7
3	L	29	ASP	2.7
3	L	127	SER	2.7
3	L	139	VAL	2.7
2	H	11	LEU	2.7
2	H	84	ALA	2.7
3	L	203	HIS	2.7
1	P	188	SER	2.7
2	H	154	GLU	2.7
2	H	215	LYS	2.7
3	L	140	CYS	2.7
2	H	125	PRO	2.7
2	H	185	SER	2.7
3	L	94	SER	2.7
2	H	122	THR	2.6
3	L	172	LYS	2.6
3	L	177	LYS	2.6
3	L	166	GLU	2.6
2	H	175	VAL	2.6
3	L	59	PRO	2.6
3	L	8	HIS	2.5
3	L	126	PRO	2.5
2	H	171	THR	2.5
1	A	192	ARG	2.5
2	H	206	HIS	2.5
2	H	126	SER	2.5
3	L	202	THR	2.5
3	L	170	PRO	2.5
3	L	152	VAL	2.5
2	H	152	PHE	2.5
3	L	93	ASP	2.4
3	L	66(A)	ASP	2.4
2	H	217	VAL	2.4
2	H	176	LEU	2.4
3	L	56	SER	2.4
2	H	180	GLY	2.3
3	L	213	ALA	2.3
3	L	67	SER	2.3
2	H	107	VAL	2.3
2	H	148	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	203	ASN	2.3
3	L	150	VAL	2.3
2	H	123	LYS	2.3
3	L	191	TRP	2.3
3	L	57	GLY	2.3
2	H	46	GLU	2.3
2	H	59	TYR	2.3
2	H	91	TYR	2.3
2	H	127	VAL	2.3
2	H	109	VAL	2.2
3	L	174	SER	2.2
2	H	145	GLY	2.2
2	H	128	PHE	2.2
2	H	147	LEU	2.2
3	L	42	ARG	2.2
2	H	61	PRO	2.2
2	H	179	SER	2.2
2	H	106	GLY	2.2
2	H	149	LYS	2.2
2	H	60	ASN	2.2
3	L	11	VAL	2.2
3	L	125	PRO	2.2
2	H	17	THR	2.2
3	L	183	TYR	2.2
2	H	108	LEU	2.2
3	L	133	ALA	2.2
3	L	103	ARG	2.1
3	L	142	ILE	2.1
2	H	63	LEU	2.1
2	H	6	GLU	2.1
3	L	66(B)	SER	2.1
3	L	134	ASN	2.1
2	H	32	TYR	2.1
2	H	96	TYR	2.1
2	H	62	SER	2.1
2	H	98	PRO	2.1
3	L	189	GLU	2.1
2	H	70	SER	2.0
2	H	75	LYS	2.0
2	H	209	SER	2.0
2	H	26	ASP	2.0
2	H	28	SER	2.0

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Mol	Chain	Res	Type	RSRZ
3	L	109	PRO	2.0
3	L	160	PRO	2.0
2	H	83	THR	2.0
2	H	150	ASP	2.0
3	L	201	VAL	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(Å ²)	Q<0.9
4	BU3	H	302	6/6	0.34	0.37	81,98,118,118	0
4	BU3	L	306	6/6	0.34	0.39	97,117,131,133	0
5	SO4	H	305	5/5	0.53	0.27	67,79,95,106	0
4	BU3	H	301	6/6	0.59	0.32	67,89,113,115	0
4	BU3	H	303	6/6	0.65	0.41	53,73,95,97	0
5	SO4	H	304	5/5	0.67	0.51	73,81,95,112	0
4	BU3	L	305	6/6	0.68	0.33	47,60,108,108	0
4	BU3	H	309	6/6	0.68	0.39	69,83,98,101	0
5	SO4	L	303	5/5	0.68	0.20	92,93,108,112	0
5	SO4	H	307	5/5	0.71	0.38	89,92,109,123	0
5	SO4	H	308	5/5	0.74	0.26	61,74,84,119	0
5	SO4	L	302	5/5	0.76	0.18	64,71,78,78	0
5	SO4	L	304	5/5	0.77	0.46	84,85,104,118	0
4	BU3	L	301	6/6	0.78	0.30	61,74,95,95	0
5	SO4	H	306	5/5	0.91	0.14	42,54,72,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.