



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 06:23 PM UTC

PDB ID : 4HWB / pdb_00004hwb
Title : Crystal structure of ectodomain 3 of the IL-13 receptor alpha 1 in complex with a human neutralizing monoclonal antibody fragment
Authors : Xu, Y.
Deposited on : 2012-11-07
Resolution : 2.61 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
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

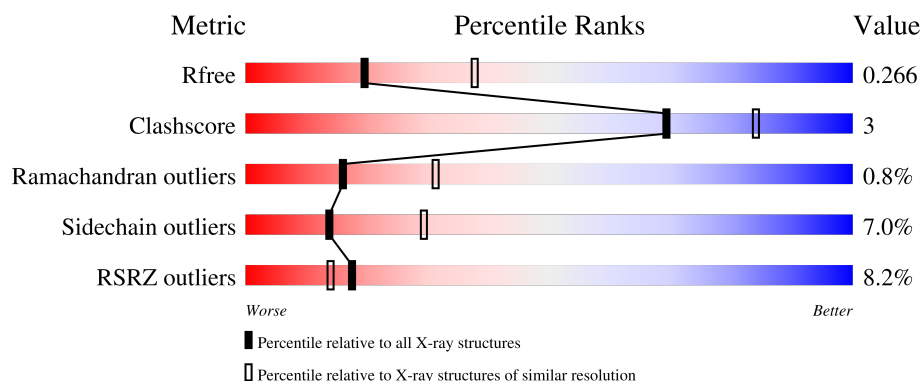
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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	122	
2	H	227	
3	L	212	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4278 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 Interleukin-13 receptor subunit alpha-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	111	Total	C	N	O	S	0	0	0
			849	540	144	160	5			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	311	HIS	-	expression tag	UNP P78552
A	312	HIS	-	expression tag	UNP P78552
A	313	HIS	-	expression tag	UNP P78552
A	314	HIS	-	expression tag	UNP P78552
A	315	HIS	-	expression tag	UNP P78552
A	316	HIS	-	expression tag	UNP P78552
A	317	HIS	-	expression tag	UNP P78552
A	318	HIS	-	expression tag	UNP P78552

- Molecule 2 is a protein called Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	216	Total	C	N	O	S	0	0	0
			1620	1035	263	314	8			

- Molecule 3 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	212	Total	C	N	O	S	0	0	0
			1602	1001	269	328	4			

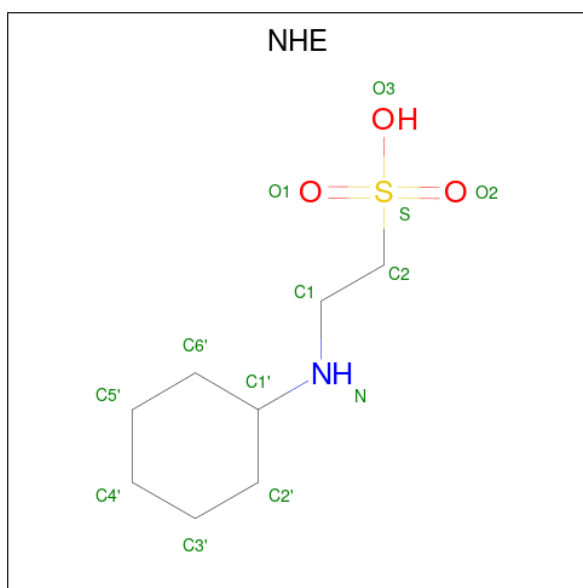
- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 5 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (CCD ID: NHE)

(formula: C₈H₁₇NO₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
5	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
5	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
5	H	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
5	H	1	Total	C	N	O	S	0	0
			13	8	1	3	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	10	Total	O	0	0
			10	10		
6	H	50	Total	O	0	0
			50	50		
6	L	17	Total	O	0	0
			17	17		

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	123.48Å 123.48Å 181.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.17 – 2.61 47.17 – 2.61	Depositor EDS
% Data completeness (in resolution range)	98.5 (47.17-2.61) 98.5 (47.17-2.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.61Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.197 , 0.224 0.229 , 0.266	Depositor DCC
R_{free} test set	2148 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	45.1	Xtriage
Anisotropy	0.531	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 74.3	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	0.93	EDS
Total number of atoms	4278	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NHE, 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	1.05	1/872 (0.1%)	1.41	9/1196 (0.8%)
2	H	0.82	1/1666 (0.1%)	1.24	3/2271 (0.1%)
3	L	0.76	1/1636 (0.1%)	1.22	7/2227 (0.3%)
All	All	0.85	3/4174 (0.1%)	1.27	19/5694 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	306	GLN	CA-C	6.48	1.60	1.52
3	L	153	SER	CA-C	5.51	1.55	1.52
2	H	154	GLU	CA-C	5.21	1.59	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	306	GLN	N-CA-C	8.79	122.84	108.52
1	A	301	TRP	CA-C-N	8.53	132.84	120.38
1	A	301	TRP	C-N-CA	8.53	132.84	120.38
1	A	242	GLN	CA-C-N	8.10	136.28	121.70
1	A	242	GLN	C-N-CA	8.10	136.28	121.70
2	H	149	LYS	N-CA-C	6.12	119.68	109.95
1	A	303	ASN	N-CA-C	5.87	118.77	110.14
1	A	222	GLU	N-CA-C	-5.83	100.75	109.15
3	L	153	SER	N-CA-C	5.80	118.04	108.48
3	L	106	THR	CB-CA-C	5.35	118.79	109.65
3	L	167	ASP	CA-CB-CG	5.33	117.93	112.60
3	L	61	ASP	CA-CB-CG	5.21	117.81	112.60
2	H	132	PRO	CA-C-N	5.10	130.88	121.70
2	H	132	PRO	C-N-CA	5.10	130.88	121.70
3	L	134	ASN	N-CA-C	5.10	118.12	109.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	291	ASN	CA-CB-CG	5.09	117.69	112.60
3	L	60	PRO	CA-C-N	5.04	127.73	120.38
3	L	60	PRO	C-N-CA	5.04	127.73	120.38
1	A	307	GLU	N-CA-C	5.03	117.44	109.50

There are no chirality outliers.

There are no planarity outliers.

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	849	0	740	7	0
2	H	1620	0	1574	14	0
3	L	1602	0	1524	10	0
4	A	10	0	0	0	0
4	H	25	0	0	0	0
4	L	30	0	0	0	0
5	A	39	0	48	2	0
5	H	26	0	32	2	0
6	A	10	0	0	0	0
6	H	50	0	0	0	0
6	L	17	0	0	0	0
All	All	4278	0	3918	28	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 (28) 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)
2:H:20:LYS:HG3	2:H:83:GLN:HB3	1.78	0.65
1:A:293:LEU:HD13	2:H:51:VAL:HG21	1.86	0.58
2:H:34:TRP:HB2	2:H:100:MET:HG3	1.85	0.58
3:L:160:VAL:HG22	3:L:172:LEU:HD12	1.85	0.57
2:H:48:TRP:CG	3:L:93:GLU:HA	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:PRO:HB3	5:A:404:NHE:H2'2	1.90	0.54
1:A:210:LEU:HD23	1:A:217:LEU:HD11	1.90	0.53
1:A:295:TYR:O	2:H:60:ARG:NH2	2.41	0.53
2:H:92:THR:HG23	2:H:116:THR:HA	1.90	0.53
2:H:19:LEU:HB2	2:H:87:LEU:HD11	1.93	0.49
1:A:224:PRO:HD2	5:A:404:NHE:HC12	1.95	0.49
1:A:249:PHE:CE1	1:A:274:PRO:HD2	2.48	0.49
2:H:60:ARG:HD2	5:H:307:NHE:O3	2.13	0.48
2:H:48:TRP:CD2	3:L:93:GLU:HA	2.47	0.48
3:L:6:GLN:H	3:L:97:GLN:HE22	1.62	0.47
3:L:178:LEU:HD13	3:L:183:TYR:HB2	1.97	0.46
2:H:37:TRP:O	2:H:49:MET:HB2	2.16	0.46
3:L:40:LYS:HE3	3:L:82:GLU:O	2.16	0.45
3:L:117:PRO:HD3	3:L:129:VAL:HG22	1.98	0.45
5:H:307:NHE:H6'2	5:H:307:NHE:HC12	1.76	0.45
3:L:48:LEU:HA	3:L:59:ILE:HG13	1.98	0.45
3:L:148:ASP:HA	3:L:188:VAL:HB	1.98	0.45
2:H:13:LYS:HD2	2:H:19:LEU:HD13	2.01	0.42
2:H:98:ALA:HB1	2:H:106:PHE:HB3	2.01	0.42
2:H:33:TYR:O	2:H:54:PRO:HD2	2.19	0.42
2:H:184:LEU:C	2:H:184:LEU:HD23	2.45	0.42
3:L:142:LYS:HB3	3:L:194:THR:HB	2.01	0.41
1:A:213:HIS:HB3	1:A:218:TYR:HE2	1.87	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	109/122 (89%)	94 (86%)	12 (11%)	3 (3%)	4	6
2	H	212/227 (93%)	205 (97%)	7 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	L	210/212 (99%)	203 (97%)	6 (3%)	1 (0%)	24	44
All	All	531/561 (95%)	502 (94%)	25 (5%)	4 (1%)	16	31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	241	SER
1	A	258	ASN
3	L	135	ASN
1	A	265	VAL

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	87/120 (72%)	83 (95%)	4 (5%)	24	47
2	H	180/193 (93%)	166 (92%)	14 (8%)	11	25
3	L	176/183 (96%)	163 (93%)	13 (7%)	13	27
All	All	443/496 (89%)	412 (93%)	31 (7%)	14	29

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	210	LEU
1	A	228	ILE
1	A	248	VAL
1	A	272	MET
2	H	14	LYS
2	H	62	SER
2	H	69	VAL
2	H	100	MET
2	H	116	THR
2	H	144	LEU
2	H	162	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	165	LEU
2	H	176	LEU
2	H	184	LEU
2	H	185	SER
2	H	198	GLN
2	H	199	THR
2	H	216	LYS
3	L	5	THR
3	L	24	ARG
3	L	30	SER
3	L	34	LEU
3	L	47	LEU
3	L	49	ILE
3	L	91	GLN
3	L	102	GLU
3	L	159	SER
3	L	174	SER
3	L	178	LEU
3	L	180	LYS
3	L	194	THR

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

Mol	Chain	Res	Type
1	A	209	ASN
1	A	220	GLN
1	A	282	ASN
3	L	91	GLN
3	L	135	ASN
3	L	144	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

18 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
4	SO4	L	302	-	4,4,4	0.26	0	6,6,6	0.17	0
5	NHE	A	405	-	13,13,13	1.54	1 (7%)	16,17,17	0.74	1 (6%)
5	NHE	A	403	-	13,13,13	2.01	1 (7%)	16,17,17	0.85	1 (6%)
5	NHE	A	404	-	13,13,13	1.58	1 (7%)	16,17,17	0.70	1 (6%)
4	SO4	A	401	-	4,4,4	0.30	0	6,6,6	0.17	0
4	SO4	L	303	-	4,4,4	0.33	0	6,6,6	0.18	0
4	SO4	L	304	-	4,4,4	0.28	0	6,6,6	0.18	0
4	SO4	H	301	-	4,4,4	0.29	0	6,6,6	0.16	0
4	SO4	H	303	-	4,4,4	0.33	0	6,6,6	0.19	0
4	SO4	L	301	-	4,4,4	0.32	0	6,6,6	0.08	0
4	SO4	L	305	-	4,4,4	0.29	0	6,6,6	0.17	0
5	NHE	H	307	-	13,13,13	1.44	1 (7%)	16,17,17	0.86	1 (6%)
4	SO4	H	305	-	4,4,4	0.31	0	6,6,6	0.15	0
4	SO4	L	306	-	4,4,4	0.31	0	6,6,6	0.18	0
5	NHE	H	306	-	13,13,13	1.20	1 (7%)	16,17,17	0.52	0
4	SO4	H	304	-	4,4,4	0.32	0	6,6,6	0.16	0
4	SO4	A	402	-	4,4,4	0.28	0	6,6,6	0.10	0
4	SO4	H	302	-	4,4,4	0.54	0	6,6,6	0.24	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
5	NHE	A	405	-	-	1/7/15/15	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NHE	A	403	-	-	1/7/15/15	0/1/1/1
5	NHE	A	404	-	-	2/7/15/15	0/1/1/1
5	NHE	H	307	-	-	2/7/15/15	0/1/1/1
5	NHE	H	306	-	-	5/7/15/15	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	403	NHE	C2-S	-7.18	1.67	1.77
5	A	404	NHE	C2-S	-5.53	1.69	1.77
5	A	405	NHE	C2-S	-5.40	1.70	1.77
5	H	307	NHE	C2-S	-4.75	1.70	1.77
5	H	306	NHE	C2-S	-3.83	1.72	1.77

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	307	NHE	C1-N-C1'	2.75	119.48	114.18
5	A	403	NHE	C6'-C1'-N	2.71	124.09	110.56
5	A	405	NHE	C6'-C1'-N	2.64	123.72	110.56
5	A	404	NHE	C2'-C1'-N	2.55	123.31	110.56

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	404	NHE	N-C1-C2-S
5	H	306	NHE	C1-C2-S-O1
5	H	307	NHE	C6'-C1'-N-C1
5	H	306	NHE	C1-C2-S-O3
5	A	404	NHE	C2-C1-N-C1'
5	A	405	NHE	C2-C1-N-C1'
5	H	306	NHE	C2'-C1'-N-C1
5	H	306	NHE	C1-C2-S-O2
5	H	306	NHE	C6'-C1'-N-C1
5	A	403	NHE	N-C1-C2-S
5	H	307	NHE	N-C1-C2-S

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	404	NHE	2	0
5	H	307	NHE	2	0

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	111/122 (90%)	1.60	32 (28%) 1 1	47, 79, 135, 145	0
2	H	216/227 (95%)	-0.06	7 (3%) 50 45	36, 54, 106, 119	0
3	L	212/212 (100%)	0.23	5 (2%) 59 54	45, 72, 103, 133	0
All	All	539/561 (96%)	0.40	44 (8%) 17 14	36, 66, 115, 145	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	260	GLU	7.9
3	L	212	ALA	7.6
1	A	241	SER	7.4
3	L	211	CYS	6.7
1	A	265	VAL	6.7
1	A	200	VAL	6.6
1	A	261	PHE	6.4
1	A	264	ASN	6.4
1	A	310	ILE	6.2
1	A	259	PRO	6.1
1	A	266	GLU	5.8
1	A	263	ARG	5.7
1	A	202	PRO	5.5
1	A	257	GLU	5.4
1	A	240	ASN	5.2
1	A	267	ASN	4.6
1	A	245	THR	4.6
1	A	244	GLU	4.5
1	A	243	THR	4.3
1	A	305	SER	4.3
1	A	201	LYS	4.2
1	A	242	GLN	4.0
1	A	258	ASN	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	1	ALA	3.6
2	H	133	SER	3.6
2	H	220	LYS	3.6
2	H	134	SER	3.4
1	A	221	TRP	3.2
1	A	309	SER	3.1
1	A	308	MET	2.9
1	A	306	GLN	2.8
1	A	246	HIS	2.8
2	H	140	GLY	2.7
2	H	141	THR	2.6
1	A	204	PRO	2.5
3	L	78	ARG	2.5
2	H	139	GLY	2.5
1	A	275	GLY	2.4
3	L	146	LYS	2.3
1	A	272	MET	2.2
1	A	298	ASP	2.1
3	L	1	GLU	2.1
1	A	222	GLU	2.0
1	A	218	TYR	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
4	SO4	L	305	5/5	0.52	0.15	167,167,168,168	0
4	SO4	H	304	5/5	0.56	0.18	151,152,153,153	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	L	302	5/5	0.63	0.12	158,158,159,159	0
4	SO4	L	304	5/5	0.64	0.17	172,173,174,174	0
4	SO4	L	303	5/5	0.64	0.12	136,136,137,137	0
4	SO4	L	301	5/5	0.66	0.17	162,162,163,164	0
4	SO4	L	306	5/5	0.66	0.15	161,161,161,162	0
4	SO4	H	301	5/5	0.72	0.10	154,154,155,155	0
4	SO4	H	305	5/5	0.77	0.17	147,148,148,149	0
4	SO4	A	402	5/5	0.80	0.09	139,139,140,140	0
5	NHE	H	307	13/13	0.80	0.23	72,79,92,93	0
4	SO4	H	303	5/5	0.82	0.11	144,144,144,144	0
4	SO4	A	401	5/5	0.83	0.12	139,140,141,142	0
5	NHE	H	306	13/13	0.89	0.17	77,85,102,105	0
4	SO4	H	302	5/5	0.89	0.11	93,95,97,98	0
5	NHE	A	405	13/13	0.90	0.20	93,98,123,123	0
5	NHE	A	404	13/13	0.96	0.11	67,70,72,72	0
5	NHE	A	403	13/13	0.97	0.09	44,48,53,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.