



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:28 AM UTC

PDB ID : 1ZHH / pdb_00001zhh
Title : Crystal Structure of the Apo Form of Vibrio Harveyi LUXP Complexed with the Periplasmic Domain of LUXQ
Authors : Neiditch, M.B.; Federle, M.J.; Miller, S.T.; Bassler, B.L.; Hughson, F.M.
Deposited on : 2005-04-25
Resolution : 1.94 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

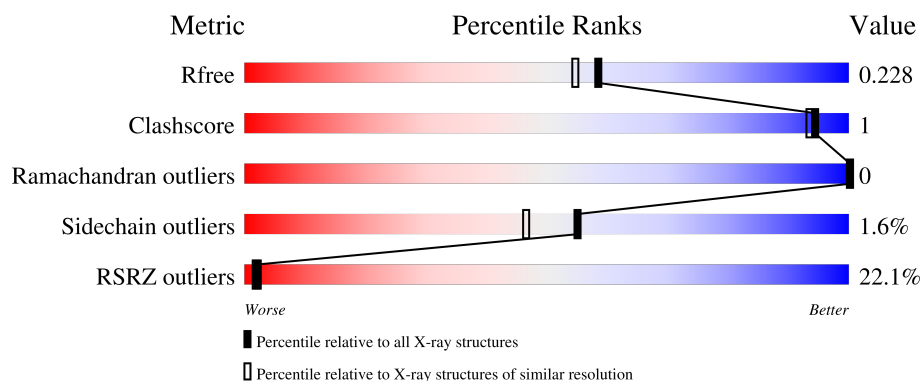
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 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	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	344	9% 97% .
2	B	242	37% 80% 6% 14%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4772 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 Autoinducer 2-binding periplasmic protein luxP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	0	0	0
			2775	1765	469	535	6			

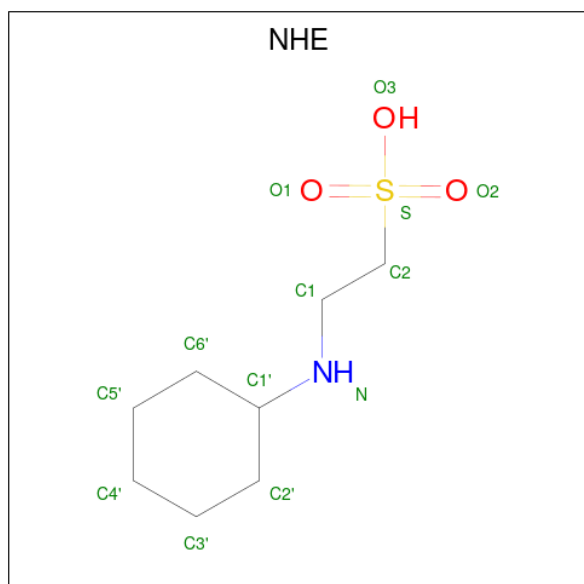
- Molecule 2 is a protein called Autoinducer 2 sensor kinase/phosphatase luxQ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	208	Total	C	N	O	S	0	0	0
			1651	1048	278	321	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	37	GLY	-	See Remark 999	UNP P54302
B	38	SER	-	See Remark 999	UNP P54302

- Molecule 3 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (CCD ID: NHE) (formula: C₈H₁₇NO₃S).



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

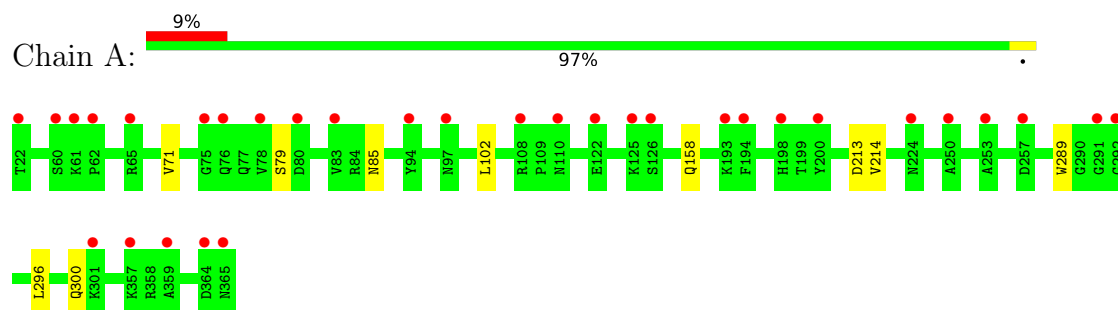
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	246	Total	O	0	0
			246	246		
4	B	87	Total	O	0	0
			87	87		

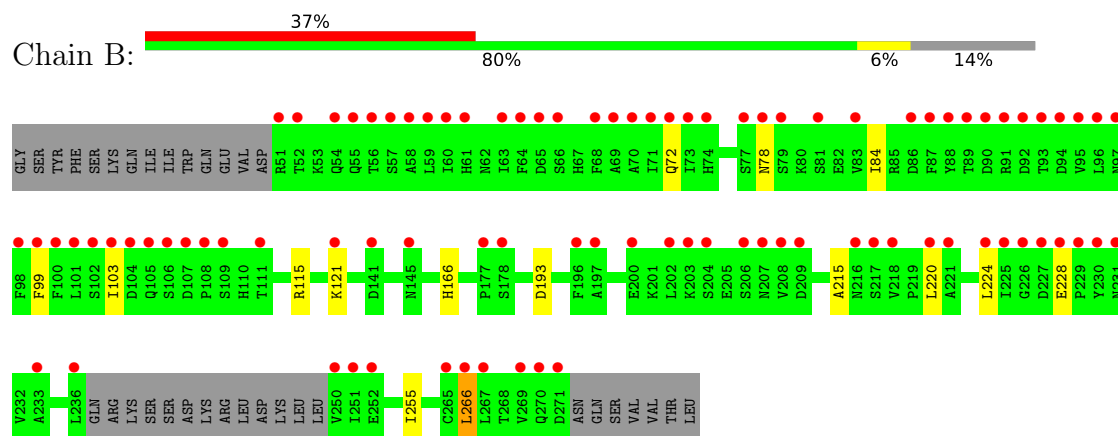
3 Residue-property plots

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: Autoinducer 2-binding periplasmic protein luxP



- Molecule 2: Autoinducer 2 sensor kinase/phosphatase luxQ



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	128.47Å 128.47Å 95.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 1.94 50.00 – 1.94	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-1.94) 96.0 (50.00-1.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.94 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.206 , 0.222 0.216 , 0.228	Depositor DCC
R_{free} test set	3245 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	35.5	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.032 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4772	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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

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	0.46	0/2840	0.75	0/3850
2	B	0.48	0/1686	0.74	0/2299
All	All	0.47	0/4526	0.74	0/6149

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

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	2775	0	2695	6	0
2	B	1651	0	1596	5	0
3	B	13	0	16	1	0
4	A	246	0	0	1	0
4	B	87	0	0	0	0
All	All	4772	0	4307	11	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 (11) 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:85:ASN:HD21	1:A:158:GLN:HE22	1.25	0.83
1:A:85:ASN:ND2	1:A:158:GLN:HE22	1.98	0.59
1:A:214:VAL:HG11	4:A:447:HOH:O	2.06	0.54
1:A:213:ASP:HB3	3:B:3256:NHE:H5'2	1.90	0.51
2:B:99:PHE:CZ	2:B:103:ILE:HD11	2.49	0.47
1:A:296:LEU:O	1:A:300:GLN:HG3	2.16	0.46
2:B:166:HIS:HD2	2:B:193:ASP:OD1	2.00	0.43
2:B:78:ASN:O	2:B:84:ILE:HD12	2.18	0.42
2:B:215:ALA:HB2	2:B:220:LEU:HD11	2.01	0.41
2:B:255:ILE:HD11	2:B:266:LEU:HD22	2.03	0.41
1:A:71:VAL:HG23	1:A:102:LEU:HD11	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	342/344 (99%)	335 (98%)	7 (2%)	0	100	100
2	B	204/242 (84%)	199 (98%)	5 (2%)	0	100	100
All	All	546/586 (93%)	534 (98%)	12 (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	299/299 (100%)	297 (99%)	2 (1%)	76	74
2	B	190/223 (85%)	184 (97%)	6 (3%)	34	20
All	All	489/522 (94%)	481 (98%)	8 (2%)	55	46

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

Mol	Chain	Res	Type
1	A	79	SER
1	A	289	TRP
2	B	72	GLN
2	B	115	ARG
2	B	121	LYS
2	B	224	LEU
2	B	228	GLU
2	B	266	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	85	ASN
1	A	224	ASN
2	B	166	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](#)

1 ligand is 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	NHE	B	3256	-	13,13,13	3.87	8 (61%)	16,17,17	3.06	8 (50%)

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	NHE	B	3256	-	-	1/7/15/15	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	3256	NHE	C1'-N	-6.08	1.31	1.48
3	B	3256	NHE	C3'-C2'	-5.90	1.38	1.53
3	B	3256	NHE	C6'-C1'	-5.61	1.39	1.52
3	B	3256	NHE	C2'-C1'	-5.44	1.39	1.52
3	B	3256	NHE	C5'-C6'	-5.26	1.40	1.53
3	B	3256	NHE	C4'-C5'	-3.31	1.39	1.51
3	B	3256	NHE	C4'-C3'	-3.21	1.40	1.51
3	B	3256	NHE	O2-S	2.26	1.51	1.45

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3256	NHE	C6'-C1'-C2'	6.56	122.13	110.80
3	B	3256	NHE	C3'-C2'-C1'	4.77	119.64	111.09
3	B	3256	NHE	C4'-C5'-C6'	4.29	120.24	111.42
3	B	3256	NHE	C5'-C6'-C1'	3.80	117.91	111.09
3	B	3256	NHE	C4'-C3'-C2'	3.73	119.08	111.42
3	B	3256	NHE	O1-S-C2	3.54	112.08	106.73
3	B	3256	NHE	C5'-C4'-C3'	3.27	120.91	111.19
3	B	3256	NHE	C6'-C1'-N	2.15	121.29	110.56

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	3256	NHE	C6'-C1'-N-C1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	3256	NHE	1	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	344/344 (100%)	0.75	32 (9%)	14 16	28, 36, 49, 62	0
2	B	208/242 (85%)	1.76	90 (43%)	0 0	32, 47, 71, 96	0
All	All	552/586 (94%)	1.13	122 (22%)	2 2	28, 38, 64, 96	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	52	THR	7.2
2	B	98	PHE	6.3
2	B	250	VAL	6.1
1	A	78	VAL	5.9
2	B	92	ASP	5.4
2	B	207	ASN	4.9
2	B	100	PHE	4.8
2	B	236	LEU	4.8
2	B	271	ASP	4.6
2	B	265	CYS	4.6
2	B	102	SER	4.3
1	A	257	ASP	4.2
2	B	204	SER	4.2
2	B	96	LEU	4.1
2	B	103	ILE	4.1
2	B	95	VAL	4.0
2	B	56	THR	3.9
2	B	101	LEU	3.7
2	B	57	SER	3.7
2	B	59	LEU	3.6
2	B	73	ILE	3.6
2	B	94	ASP	3.5
2	B	77	SER	3.5
2	B	269	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	177	PRO	3.5
1	A	365	ASN	3.5
2	B	87	PHE	3.5
2	B	224	LEU	3.4
2	B	197	ALA	3.3
2	B	68	PHE	3.3
1	A	94	TYR	3.3
2	B	93	THR	3.3
2	B	227	ASP	3.3
2	B	97	ASN	3.3
2	B	251	ILE	3.2
2	B	60	ILE	3.2
1	A	76	GLN	3.2
2	B	54	GLN	3.2
2	B	51	ARG	3.2
1	A	253	ALA	3.1
2	B	108	PRO	3.1
1	A	194	PHE	3.0
2	B	74	HIS	3.0
2	B	203	LYS	3.0
2	B	228	GLU	2.9
2	B	107	ASP	2.9
2	B	196	PHE	2.8
1	A	110	ASN	2.8
2	B	63	ILE	2.8
2	B	104	ASP	2.8
2	B	83	VAL	2.8
2	B	55	GLN	2.8
1	A	75	GLY	2.8
2	B	226	GLY	2.7
2	B	78	ASN	2.6
2	B	91	ARG	2.6
2	B	61	HIS	2.6
2	B	58	ALA	2.6
2	B	72	GLN	2.5
2	B	105	GLN	2.5
1	A	62	PRO	2.5
2	B	65	ASP	2.5
1	A	83	VAL	2.5
2	B	230	TYR	2.5
2	B	81	SER	2.5
1	A	125	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	216	ASN	2.4
1	A	198	HIS	2.4
2	B	267	LEU	2.4
2	B	70	ALA	2.4
2	B	121	LYS	2.4
2	B	90	ASP	2.4
2	B	202	LEU	2.4
1	A	193	LYS	2.4
2	B	225	ILE	2.4
1	A	97	ASN	2.4
1	A	60	SER	2.4
2	B	66	SER	2.4
2	B	106	SER	2.4
1	A	364	ASP	2.4
2	B	218	VAL	2.4
2	B	206	SER	2.4
1	A	61	LYS	2.4
2	B	89	THR	2.3
2	B	200	GLU	2.3
1	A	357	LYS	2.3
2	B	79	SER	2.3
2	B	109	SER	2.3
2	B	266	LEU	2.3
2	B	88	TYR	2.3
1	A	224	ASN	2.3
1	A	122	GLU	2.3
2	B	141	ASP	2.3
2	B	231	ASN	2.3
2	B	220	LEU	2.3
2	B	233	ALA	2.2
2	B	217	SER	2.2
2	B	99	PHE	2.2
2	B	145	ASN	2.2
2	B	252	GLU	2.2
1	A	292	GLY	2.2
1	A	22	THR	2.2
1	A	291	GLY	2.2
2	B	86	ASP	2.1
2	B	209	ASP	2.1
1	A	126	SER	2.1
2	B	71	ILE	2.1
2	B	178	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	64	PHE	2.1
2	B	229	PRO	2.1
2	B	270	GLN	2.1
1	A	359	ALA	2.1
2	B	221	ALA	2.1
1	A	301	LYS	2.0
2	B	208	VAL	2.0
1	A	65	ARG	2.0
1	A	80	ASP	2.0
1	A	108	ARG	2.0
1	A	250	ALA	2.0
2	B	69	ALA	2.0
2	B	111	THR	2.0
1	A	200	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
3	NHE	B	3256	13/13	0.70	0.20	41,44,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.