



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 09:29 AM UTC

PDB ID : 2NPE / pdb_00002npe
Title : An unusual twin-His arrangement in the pore of ammonia channels is essential for substrate conductance
Authors : Lupo, D.; Winkler, F.K.
Deposited on : 2006-10-27
Resolution : 2.10 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

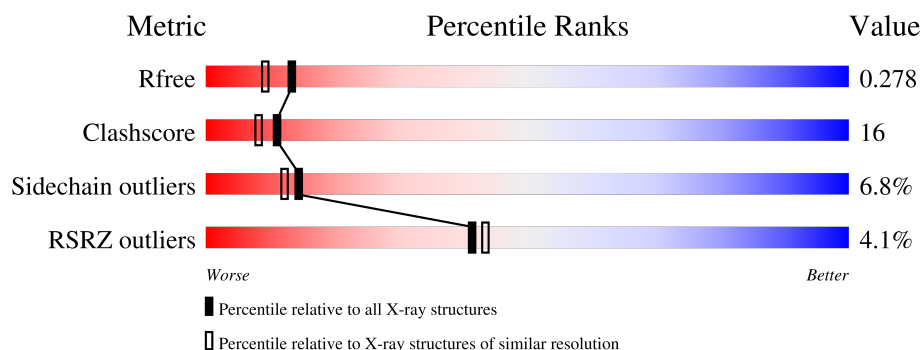
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	424	4% 57% 25% 5% 13%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2750 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 Ammonia channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	0	0	0
			2670	1768	429	454	19			

There are 19 discrepancies between the modelled and reference sequences:

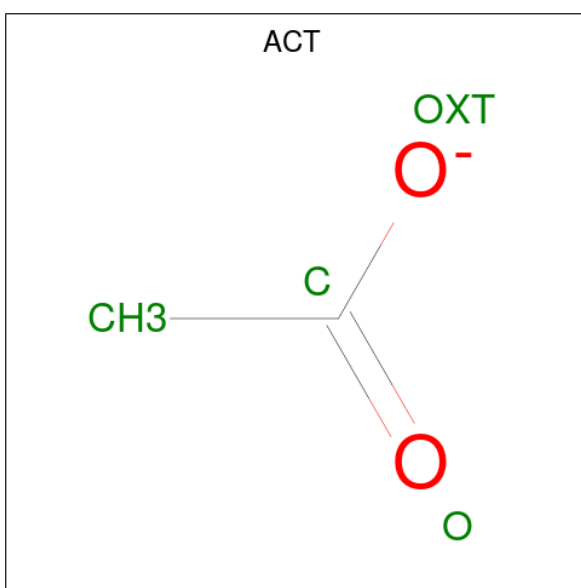
Chain	Residue	Modelled	Actual	Comment	Reference
A	318	ALA	HIS	engineered mutation	UNP P69681
A	407	ASP	-	expression tag	UNP P69681
A	408	GLN	-	expression tag	UNP P69681
A	409	ALA	-	expression tag	UNP P69681
A	410	GLN	-	expression tag	UNP P69681
A	411	GLN	-	expression tag	UNP P69681
A	412	PRO	-	expression tag	UNP P69681
A	413	ALA	-	expression tag	UNP P69681
A	414	GLN	-	expression tag	UNP P69681
A	415	ALA	-	expression tag	UNP P69681
A	416	ASP	-	expression tag	UNP P69681
A	417	LEU	-	expression tag	UNP P69681
A	418	GLU	-	expression tag	UNP P69681
A	419	HIS	-	expression tag	UNP P69681
A	420	HIS	-	expression tag	UNP P69681
A	421	HIS	-	expression tag	UNP P69681
A	422	HIS	-	expression tag	UNP P69681
A	423	HIS	-	expression tag	UNP P69681
A	424	HIS	-	expression tag	UNP P69681

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	66	Total 66	O 66	0	0

- Molecule 1: Ammonia channel



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	109.25Å 109.25Å 84.39Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.10 15.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (15.00-2.10) 98.8 (15.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.211 , 0.254 (Not available) , 0.278	Depositor DCC
R_{free} test set	1670 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.448	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 69.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.060 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2750	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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: ACT, 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	1.18	7/2731 (0.3%)	1.25	19/3723 (0.5%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	242	ILE	CA-CB	-8.45	1.45	1.54
1	A	286	ILE	CA-CB	-7.27	1.45	1.54
1	A	252	LEU	CG-CD2	6.56	1.74	1.52
1	A	207	ILE	CA-CB	-5.72	1.47	1.54
1	A	281	VAL	CA-C	5.38	1.59	1.52
1	A	211	GLY	N-CA	5.29	1.52	1.45
1	A	61	VAL	N-CA	5.07	1.52	1.46

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	93	GLY	N-CA-C	-10.88	101.66	111.67
1	A	235	VAL	N-CA-C	-9.24	101.84	110.53
1	A	269	LEU	N-CA-C	-7.47	103.08	111.14
1	A	281	VAL	N-CA-C	-6.66	101.98	111.17
1	A	15	ILE	N-CA-C	-6.61	104.07	110.42
1	A	242	ILE	CB-CA-C	-6.58	103.46	111.88
1	A	218	GLY	N-CA-C	-6.12	106.16	113.99
1	A	332	PHE	N-CA-C	5.56	119.16	112.38
1	A	204	GLY	N-CA-C	-5.52	105.81	112.49
1	A	177	VAL	N-CA-C	-5.32	105.19	110.62
1	A	273	THR	CA-C-N	-5.31	114.35	119.87
1	A	273	THR	C-N-CA	-5.31	114.35	119.87
1	A	211	GLY	N-CA-C	-5.30	106.26	113.37
1	A	246	ILE	N-CA-C	5.28	115.90	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	281	VAL	CB-CA-C	-5.26	104.37	112.05
1	A	279	ILE	CA-C-N	5.26	125.33	120.34
1	A	279	ILE	C-N-CA	5.26	125.33	120.34
1	A	68	PHE	N-CA-C	5.23	119.79	113.41
1	A	57	ILE	CB-CA-C	-5.01	105.53	112.24

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	2670	0	2747	88	0
2	A	10	0	0	1	0
3	A	4	0	3	1	0
4	A	66	0	0	5	0
All	All	2750	0	2750	89	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 16.

All (89) 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:300:THR:O	1:A:303:LYS:HD2	1.41	1.18
1:A:37:ARG:HD3	4:A:663:HOH:O	1.63	0.96
1:A:385:VAL:HG12	1:A:386:PRO:HD2	1.49	0.92
1:A:125:PHE:O	1:A:128:VAL:HG12	1.82	0.79
1:A:295:GLY:HA3	4:A:660:HOH:O	1.83	0.77
1:A:301:MET:HE3	1:A:301:MET:HA	1.71	0.73
1:A:130:ILE:HD13	1:A:380:THR:HG21	1.71	0.72
1:A:236:VAL:CG1	1:A:285:LEU:HB2	2.20	0.72
1:A:143:ILE:HA	1:A:146:MET:HE3	1.76	0.66
1:A:130:ILE:HD13	1:A:380:THR:CG2	2.25	0.65
1:A:65:SER:HB2	1:A:80:TRP:HB2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:VAL:HG23	1:A:282:GLY:N	2.13	0.62
1:A:371:PHE:CZ	1:A:375:LYS:HE3	2.35	0.61
1:A:281:VAL:O	1:A:282:GLY:C	2.44	0.60
1:A:57:ILE:O	1:A:61:VAL:HG23	2.01	0.59
1:A:377:ALA:HA	1:A:380:THR:HG22	1.85	0.59
1:A:384:ARG:HD3	1:A:384:ARG:H	1.70	0.56
1:A:127:ALA:HB1	1:A:383:LEU:HD23	1.87	0.56
1:A:124:ARG:O	1:A:127:ALA:HB3	2.05	0.55
1:A:67:ALA:O	1:A:145:HIS:ND1	2.36	0.54
1:A:303:LYS:O	1:A:303:LYS:HD3	2.07	0.54
1:A:246:ILE:HG23	1:A:256:PRO:HB3	1.89	0.54
1:A:310:ASP:C	1:A:312:CYS:H	2.16	0.53
1:A:371:PHE:CE2	1:A:375:LYS:HG3	2.44	0.52
1:A:275:ALA:HB2	1:A:329:THR:OG1	2.09	0.52
1:A:65:SER:CB	1:A:80:TRP:HB2	2.39	0.52
1:A:377:ALA:O	1:A:380:THR:HG22	2.10	0.52
1:A:335:SER:O	1:A:336:SER:C	2.53	0.51
1:A:169:ILE:O	1:A:173:ILE:HG12	2.11	0.51
1:A:180:TYR:CG	1:A:180:TYR:O	2.64	0.50
1:A:380:THR:CG2	1:A:381:VAL:N	2.75	0.50
1:A:209:TYR:O	1:A:210:ILE:C	2.50	0.50
1:A:125:PHE:O	1:A:128:VAL:N	2.45	0.49
1:A:310:ASP:N	1:A:312:CYS:H	2.10	0.49
1:A:60:VAL:HG12	1:A:82:MET:SD	2.52	0.49
1:A:281:VAL:CG2	1:A:282:GLY:N	2.76	0.49
1:A:249:GLU:OE1	1:A:260:GLY:HA3	2.12	0.48
1:A:36:ILE:O	1:A:196:HIS:ND1	2.45	0.48
1:A:124:ARG:HG3	2:A:501:SO4:O2	2.14	0.48
1:A:235:VAL:O	1:A:236:VAL:C	2.55	0.47
1:A:33:GLY:O	1:A:196:HIS:CE1	2.68	0.47
1:A:232:VAL:HG12	1:A:281:VAL:HG12	1.97	0.47
1:A:36:ILE:HG22	1:A:311:PRO:HG3	1.96	0.47
1:A:62:TYR:C	1:A:62:TYR:CD1	2.93	0.46
1:A:353:LEU:HD13	1:A:353:LEU:HA	1.78	0.46
1:A:200:MET:HE3	1:A:200:MET:HB2	1.84	0.45
1:A:311:PRO:O	1:A:314:VAL:HG23	2.16	0.45
1:A:323:ILE:O	1:A:327:ILE:HG13	2.16	0.45
3:A:601:ACT:H1	4:A:644:HOH:O	2.16	0.45
1:A:267:ALA:CB	4:A:660:HOH:O	2.64	0.45
1:A:212:TRP:CE3	1:A:269:LEU:HD13	2.52	0.45
1:A:36:ILE:HD11	1:A:41:VAL:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:LYS:O	1:A:303:LYS:CD	2.65	0.45
1:A:264:GLY:O	1:A:265:ALA:C	2.58	0.44
1:A:123:ILE:CG2	1:A:128:VAL:HB	2.47	0.44
1:A:285:LEU:C	1:A:285:LEU:HD23	2.42	0.44
1:A:320:VAL:O	1:A:324:VAL:HG23	2.17	0.44
1:A:6:ASP:C	1:A:6:ASP:OD1	2.61	0.44
1:A:147:VAL:HG22	1:A:153:LEU:HD12	2.00	0.43
1:A:28:ILE:HD13	1:A:114:LEU:HD23	2.00	0.43
1:A:301:MET:HA	1:A:301:MET:CE	2.45	0.43
1:A:383:LEU:HD23	1:A:383:LEU:HA	1.80	0.43
1:A:197:ASN:ND2	1:A:200:MET:HE3	2.33	0.43
1:A:84:LYS:HD2	1:A:84:LYS:HA	1.67	0.43
1:A:267:ALA:HB1	4:A:660:HOH:O	2.17	0.43
1:A:319:GLY:O	1:A:323:ILE:HG13	2.19	0.43
1:A:165:THR:O	1:A:170:ASN:HB2	2.19	0.43
1:A:266:ILE:HA	1:A:266:ILE:HD13	1.81	0.43
1:A:242:ILE:O	1:A:246:ILE:HG12	2.18	0.43
1:A:380:THR:HG23	1:A:381:VAL:N	2.34	0.43
1:A:236:VAL:HG12	1:A:285:LEU:HB2	1.99	0.42
1:A:364:VAL:O	1:A:368:VAL:HG23	2.19	0.42
1:A:24:THR:HA	1:A:28:ILE:HG22	2.01	0.42
1:A:120:ALA:O	1:A:121:GLU:C	2.62	0.42
1:A:302:LEU:HD23	1:A:302:LEU:HA	1.90	0.42
1:A:173:ILE:HG13	1:A:363:ILE:HA	2.02	0.41
1:A:237:ALA:CB	1:A:272:VAL:HB	2.50	0.41
1:A:350:HIS:O	1:A:351:GLN:C	2.60	0.41
1:A:42:LEU:HD23	1:A:42:LEU:HA	1.93	0.41
1:A:203:THR:O	1:A:206:ALA:HB3	2.20	0.41
1:A:384:ARG:H	1:A:384:ARG:CD	2.30	0.41
1:A:124:ARG:HD2	1:A:382:GLY:O	2.21	0.41
1:A:37:ARG:HG3	1:A:39:LYS:HG2	2.03	0.41
1:A:61:VAL:O	1:A:81:LEU:HA	2.21	0.41
1:A:137:THR:HA	1:A:141:ILE:HD12	2.02	0.41
1:A:288:GLY:O	1:A:289:VAL:C	2.63	0.41
1:A:233:ASN:O	1:A:234:THR:C	2.64	0.40
1:A:141:ILE:HB	1:A:142:PRO:HD3	2.03	0.40
1:A:161:PHE:HB2	1:A:278:TYR:CE2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	266/311 (86%)	248 (93%)	18 (7%)	14	12

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	VAL
1	A	26	PRO
1	A	28	ILE
1	A	70	GLU
1	A	81	LEU
1	A	92	MET
1	A	123	ILE
1	A	207	ILE
1	A	210	ILE
1	A	255	LYS
1	A	273	THR
1	A	285	LEU
1	A	301	MET
1	A	303	LYS
1	A	336	SER
1	A	380	THR
1	A	384	ARG
1	A	385	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	ASN
1	A	350	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](#)

3 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	$\# Z > 2$
2	SO4	A	503	-	4,4,4	0.28	0	6,6,6	0.30	0
3	ACT	A	601	-	3,3,3	0.75	0	3,3,3	1.25	0
2	SO4	A	501	-	4,4,4	0.24	0	6,6,6	0.27	0

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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	ACT	1	0
2	A	501	SO4	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	367/424 (86%)	0.36	15 (4%)	41 43	21, 33, 56, 81	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	344	GLU	4.1
1	A	196	HIS	2.9
1	A	374	TYR	2.8
1	A	79	ASN	2.7
1	A	377	ALA	2.7
1	A	375	LYS	2.5
1	A	379	LEU	2.4
1	A	180	TYR	2.3
1	A	253	ARG	2.3
1	A	75	PHE	2.3
1	A	209	TYR	2.3
1	A	381	VAL	2.2
1	A	252	LEU	2.2
1	A	353	LEU	2.2
1	A	303	LYS	2.1

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
2	SO4	A	503	5/5	0.67	0.16	150,152,153,154	0
2	SO4	A	501	5/5	0.77	0.16	124,124,125,126	0
3	ACT	A	601	4/4	0.83	0.11	64,65,65,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.