



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:55 PM UTC

PDB ID : 5FHY / pdb_00005fhy
Title : Crystal structure of FliD (HAP2) from Pseudomonas aeruginosa PAO1
Authors : Postel, S.; Bonsor, D.; Diederichs, K.; Sundberg, E.J.
Deposited on : 2015-12-22
Resolution : 2.20 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

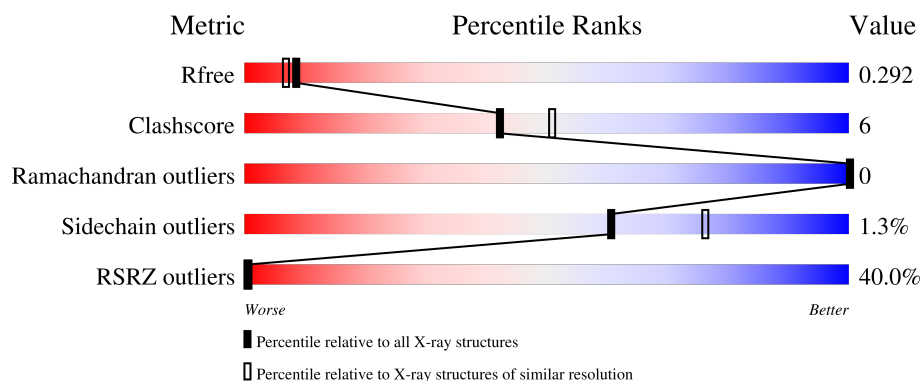
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	346	20% 57% 10% 34%
1	B	346	33% 53% 13% 34%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3219 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 B-type flagellar hook-associated protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	0	0
			1569	962	271	335	1			
1	B	229	Total	C	N	O	S	0	0	0
			1559	957	269	332	1			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	MET	-	expression tag	UNP Q9K3C5
A	61	GLY	-	expression tag	UNP Q9K3C5
A	62	HIS	-	expression tag	UNP Q9K3C5
A	63	HIS	-	expression tag	UNP Q9K3C5
A	64	HIS	-	expression tag	UNP Q9K3C5
A	65	HIS	-	expression tag	UNP Q9K3C5
A	66	HIS	-	expression tag	UNP Q9K3C5
A	67	HIS	-	expression tag	UNP Q9K3C5
A	68	GLY	-	expression tag	UNP Q9K3C5
A	69	GLY	-	expression tag	UNP Q9K3C5
A	70	SER	-	expression tag	UNP Q9K3C5
A	71	GLU	-	expression tag	UNP Q9K3C5
A	72	ASN	-	expression tag	UNP Q9K3C5
A	73	LEU	-	expression tag	UNP Q9K3C5
A	74	TYR	-	expression tag	UNP Q9K3C5
A	75	PHE	-	expression tag	UNP Q9K3C5
A	76	GLN	-	expression tag	UNP Q9K3C5
A	77	GLY	-	expression tag	UNP Q9K3C5
B	60	MET	-	expression tag	UNP Q9K3C5
B	61	GLY	-	expression tag	UNP Q9K3C5
B	62	HIS	-	expression tag	UNP Q9K3C5
B	63	HIS	-	expression tag	UNP Q9K3C5
B	64	HIS	-	expression tag	UNP Q9K3C5
B	65	HIS	-	expression tag	UNP Q9K3C5
B	66	HIS	-	expression tag	UNP Q9K3C5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	67	HIS	-	expression tag	UNP Q9K3C5
B	68	GLY	-	expression tag	UNP Q9K3C5
B	69	GLY	-	expression tag	UNP Q9K3C5
B	70	SER	-	expression tag	UNP Q9K3C5
B	71	GLU	-	expression tag	UNP Q9K3C5
B	72	ASN	-	expression tag	UNP Q9K3C5
B	73	LEU	-	expression tag	UNP Q9K3C5
B	74	TYR	-	expression tag	UNP Q9K3C5
B	75	PHE	-	expression tag	UNP Q9K3C5
B	76	GLN	-	expression tag	UNP Q9K3C5
B	77	GLY	-	expression tag	UNP Q9K3C5

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0
2	B	2	Total Na 2 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	55	Total O 55 55	0	0
3	B	33	Total O 33 33	0	0

ILE

4 Data and refinement statistics

Property	Value	Source
Space group	P 6	Depositor
Cell constants a, b, c, α , β , γ	124.74Å 124.74Å 107.01Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	62.37 – 2.20 62.37 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.8 (62.37-2.20) 97.7 (62.37-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.249 , 0.287 0.263 , 0.292	Depositor DCC
R_{free} test set	2306 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	61.0	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 70.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.053 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3219	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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: NA

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	0.35	0/1579	0.84	7/2148 (0.3%)
1	B	0.33	0/1570	0.79	3/2139 (0.1%)
All	All	0.34	0/3149	0.82	10/4287 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	251	VAL	N-CA-C	-6.59	104.34	110.53
1	A	281	LYS	N-CA-C	-6.36	105.01	112.89
1	B	210	ASP	CA-C-N	6.01	125.69	119.56
1	B	210	ASP	C-N-CA	6.01	125.69	119.56
1	A	295	THR	N-CA-C	-5.60	107.10	114.04
1	A	275	ARG	N-CA-C	-5.51	106.51	113.18
1	A	210	ASP	CA-C-N	5.41	125.08	119.56
1	A	210	ASP	C-N-CA	5.41	125.08	119.56
1	B	251	VAL	N-CA-C	-5.28	105.39	110.72
1	A	278	ALA	N-CA-C	-5.14	107.17	112.93

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	305	THR	Peptide

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	1569	0	1534	14	0
1	B	1559	0	1506	25	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
3	A	55	0	0	1	0
3	B	33	0	0	0	0
All	All	3219	0	3040	39	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 6.

All (39) 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:SER:HB3	1:A:257:PHE:HB3	1.72	0.72
1:B:297:PHE:HA	1:B:301:GLN:HB2	1.74	0.70
1:A:82:LEU:HD12	1:A:269:ILE:HD11	1.74	0.69
1:A:286:LYS:O	1:A:290:ALA:N	2.22	0.66
1:B:159:LYS:NZ	1:B:160:GLU:OE1	2.29	0.62
1:B:289:GLU:O	1:B:293:THR:N	2.25	0.59
1:A:216:LYS:NZ	3:A:604:HOH:O	2.29	0.58
1:A:132:ASP:OD1	1:A:133:THR:N	2.36	0.58
1:B:168:ILE:HD12	1:B:177:VAL:HG21	1.87	0.57
1:A:168:ILE:HD12	1:A:177:VAL:HG21	1.85	0.56
1:A:247:SER:OG	1:A:258:ASP:OD1	2.22	0.56
1:B:104:THR:OG1	1:B:228:LYS:O	2.28	0.51
1:B:156:GLN:O	1:B:159:LYS:NZ	2.35	0.49
1:B:141:ASP:OD1	1:B:143:SER:OG	2.22	0.49
1:A:155:ASN:OD1	1:A:165:ALA:N	2.45	0.49
1:A:277:ASP:C	1:A:279:GLY:H	2.20	0.48
1:B:247:SER:OG	1:B:258:ASP:OD1	2.20	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:LEU:HD12	1:B:269:ILE:HD11	1.97	0.47
1:B:153:ALA:O	1:B:157:ALA:N	2.46	0.46
1:A:83:LYS:HZ2	1:A:97:ILE:HD12	1.80	0.45
1:A:306:LYS:HG3	1:A:307:VAL:N	2.31	0.45
1:B:83:LYS:NZ	1:B:97:ILE:HD12	2.31	0.45
1:A:83:LYS:HB3	1:A:83:LYS:HE2	1.54	0.45
1:B:225:TYR:CE1	1:B:228:LYS:HG2	2.52	0.44
1:B:83:LYS:HB3	1:B:83:LYS:HE2	1.57	0.44
1:B:110:LEU:HD12	1:B:176:LEU:HB2	1.99	0.43
1:B:99:VAL:O	1:B:262:VAL:HG13	2.19	0.43
1:B:80:ASP:N	1:B:80:ASP:OD1	2.52	0.43
1:B:279:GLY:HA2	1:B:280:VAL:HA	1.64	0.42
1:B:85:SER:HB3	1:B:257:PHE:HB3	2.01	0.42
1:A:266:GLY:C	1:A:267:LYS:HD3	2.44	0.42
1:B:112:ALA:HA	1:B:175:ARG:HB3	2.02	0.42
1:B:235:THR:HG22	1:B:240:LYS:HG2	2.01	0.42
1:A:80:ASP:N	1:A:80:ASP:OD1	2.51	0.42
1:B:126:LEU:HB2	1:B:138:ILE:HB	2.01	0.41
1:B:132:ASP:OD1	1:B:132:ASP:C	2.63	0.41
1:B:80:ASP:CG	1:B:81:ILE:H	2.28	0.41
1:B:148:ALA:HB1	1:B:151:ARG:HH21	1.86	0.40
1:B:154:ILE:HD13	1:B:178:LEU:HD21	2.02	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	227/346 (66%)	213 (94%)	14 (6%)	0	100	100
1	B	227/346 (66%)	213 (94%)	14 (6%)	0	100	100
All	All	454/692 (66%)	426 (94%)	28 (6%)	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	161/272 (59%)	159 (99%)	2 (1%)	63	78
1	B	157/272 (58%)	155 (99%)	2 (1%)	61	76
All	All	318/544 (58%)	314 (99%)	4 (1%)	61	76

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	ILE
1	A	130	VAL
1	B	130	VAL
1	B	159	LYS

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	96	GLN
1	A	127	ASN
1	B	96	GLN
1	B	127	ASN

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](#)

Of 3 ligands modelled in this entry, 3 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 [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	229/346 (66%)	1.56	69 (30%) 1 1	50, 75, 161, 208	0
1	B	229/346 (66%)	2.12	114 (49%) 0 0	65, 94, 163, 221	0
All	All	458/692 (66%)	1.84	183 (39%) 1 0	50, 84, 165, 221	0

All (183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	276	ASP	8.2
1	B	81	ILE	6.1
1	A	81	ILE	5.7
1	A	90	ALA	5.6
1	B	280	VAL	5.6
1	A	275	ARG	5.4
1	B	90	ALA	5.3
1	B	262	VAL	5.2
1	B	287	PHE	5.2
1	B	308	GLY	5.1
1	B	89	SER	4.7
1	B	205	SER	4.7
1	B	302	THR	4.7
1	B	195	ASP	4.6
1	B	277	ASP	4.6
1	A	298	ILE	4.6
1	B	121	PHE	4.5
1	A	308	GLY	4.5
1	A	80	ASP	4.4
1	A	87	THR	4.4
1	A	293	THR	4.4
1	A	294	LEU	4.4
1	A	283	ASN	4.4
1	B	267	LYS	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	201	ASN	4.2
1	A	284	VAL	4.2
1	B	84	ALA	4.1
1	A	303	VAL	4.1
1	B	276	ASP	4.1
1	B	112	ALA	4.0
1	A	280	VAL	3.9
1	A	91	VAL	3.9
1	B	117	ALA	3.9
1	A	132	ASP	3.9
1	B	204	LEU	3.8
1	B	87	THR	3.8
1	A	89	SER	3.8
1	A	299	ASN	3.7
1	B	114	ALA	3.7
1	B	93	GLY	3.7
1	B	126	LEU	3.7
1	B	165	ALA	3.7
1	A	297	PHE	3.6
1	B	132	ASP	3.6
1	B	282	ASP	3.6
1	B	305	THR	3.6
1	B	273	VAL	3.6
1	A	302	THR	3.6
1	A	292	ASN	3.5
1	B	80	ASP	3.5
1	A	204	LEU	3.5
1	B	291	TYR	3.4
1	A	281	LYS	3.4
1	B	253	ASP	3.4
1	B	294	LEU	3.4
1	B	133	THR	3.3
1	A	83	LYS	3.3
1	B	248	VAL	3.3
1	B	297	PHE	3.3
1	B	91	VAL	3.3
1	B	192	GLU	3.2
1	A	189	ILE	3.2
1	B	108	ILE	3.2
1	B	194	SER	3.2
1	A	290	ALA	3.2
1	B	278	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	135	LEU	3.2
1	B	202	THR	3.2
1	B	259	VAL	3.2
1	B	94	THR	3.1
1	B	299	ASN	3.1
1	A	82	LEU	3.1
1	B	168	ILE	3.1
1	B	189	ILE	3.1
1	B	92	ALA	3.1
1	B	83	LYS	3.1
1	B	288	VAL	3.1
1	B	271	LEU	3.1
1	A	134	LYS	3.0
1	B	138	ILE	3.0
1	B	137	ALA	3.0
1	B	214	ALA	3.0
1	B	82	LEU	3.0
1	A	117	ALA	2.9
1	B	207	LEU	2.9
1	B	208	ALA	2.9
1	B	264	GLU	2.9
1	A	288	VAL	2.9
1	B	128	ILE	2.8
1	B	266	GLY	2.8
1	B	298	ILE	2.8
1	A	307	VAL	2.8
1	B	284	VAL	2.8
1	A	269	ILE	2.8
1	B	154	ILE	2.8
1	A	147	LEU	2.8
1	B	113	ILE	2.7
1	B	213	THR	2.7
1	A	260	LYS	2.7
1	B	102	LEU	2.7
1	A	84	ALA	2.7
1	A	291	TYR	2.7
1	B	209	PHE	2.6
1	A	258	ASP	2.6
1	B	166	THR	2.6
1	A	207	LEU	2.6
1	A	193	VAL	2.6
1	A	295	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	167	ILE	2.6
1	A	167	ILE	2.6
1	B	190	LYS	2.6
1	B	147	LEU	2.6
1	B	139	THR	2.6
1	A	155	ASN	2.5
1	A	279	GLY	2.5
1	B	140	VAL	2.5
1	A	160	GLU	2.5
1	A	289	GLU	2.5
1	B	150	MET	2.5
1	B	199	GLY	2.5
1	A	130	VAL	2.5
1	B	307	VAL	2.5
1	A	208	ALA	2.5
1	A	278	ALA	2.5
1	B	122	ASN	2.5
1	A	287	PHE	2.5
1	B	191	VAL	2.5
1	B	95	TYR	2.5
1	A	282	ASP	2.5
1	A	156	GLN	2.5
1	B	149	GLY	2.5
1	B	203	SER	2.4
1	A	150	MET	2.4
1	B	127	ASN	2.4
1	A	121	PHE	2.4
1	B	275	ARG	2.4
1	A	131	GLY	2.3
1	A	306	LYS	2.3
1	B	162	GLY	2.3
1	B	187	LYS	2.3
1	B	125	THR	2.3
1	A	142	SER	2.3
1	B	286	LYS	2.3
1	B	109	ALA	2.3
1	B	272	THR	2.3
1	A	127	ASN	2.3
1	B	211	PRO	2.3
1	B	229	ALA	2.3
1	A	273	VAL	2.3
1	B	193	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	160	GLU	2.3
1	A	198	SER	2.2
1	B	101	SER	2.2
1	B	188	ASP	2.2
1	B	293	THR	2.2
1	B	178	LEU	2.2
1	B	257	PHE	2.2
1	A	151	ARG	2.2
1	B	186	GLY	2.2
1	A	88	GLN	2.2
1	A	139	THR	2.2
1	A	305	THR	2.2
1	A	154	ILE	2.2
1	A	201	ASN	2.2
1	B	279	GLY	2.2
1	A	85	SER	2.2
1	B	129	SER	2.2
1	B	223	ALA	2.2
1	A	262	VAL	2.1
1	B	200	GLY	2.1
1	A	161	ALA	2.1
1	B	106	SER	2.1
1	B	290	ALA	2.1
1	A	209	PHE	2.1
1	B	161	ALA	2.0
1	B	144	ASN	2.0
1	B	155	ASN	2.0
1	B	258	ASP	2.0
1	B	252	ILE	2.0
1	B	228	LYS	2.0
1	B	111	GLN	2.0
1	B	100	ASN	2.0
1	B	268	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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	NA	B	501	1/1	0.96	0.09	71,71,71,71	0
2	NA	A	501	1/1	0.97	0.13	65,65,65,65	0
2	NA	B	502	1/1	0.99	0.12	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.