



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:32 PM GMT

PDB ID : 4LZ9
Title : Structure of MATE multidrug transporter DinF-BH in complex with R6G
Authors : Lu, M.; Radchenko, M.; Symersky, J.; Nie, R.; Guo, Y.
Deposited on : 2013-07-31
Resolution : 3.70 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

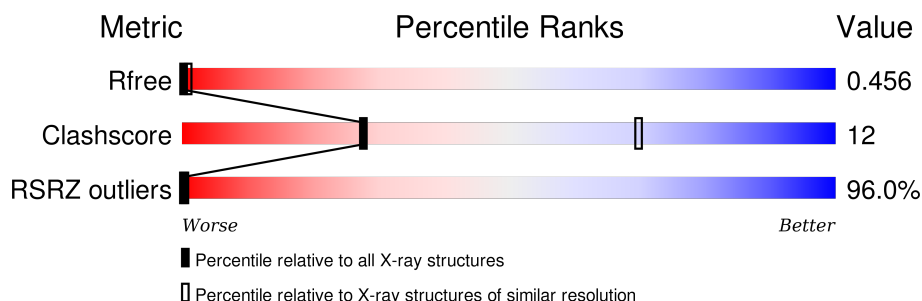
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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}	91344	1101 (3.90-3.50)
Clashscore	102246	1224 (3.90-3.50)
RSRZ outliers	91569	1108 (3.90-3.50)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	446	<div> <div>96%</div> <div>100%</div> </div>

2 Entry composition [i](#)

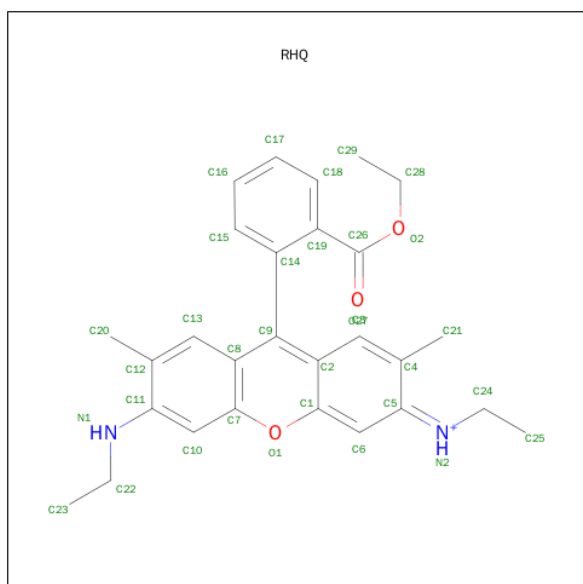
There are 2 unique types of molecules in this entry. The entry contains 479 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BH2163 protein.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
1	A	446	Total	C		0	0	446
			446	446				

- Molecule 2 is RHODAMINE 6G (three-letter code: RHQ) (formula: $C_{28}H_{31}N_2O_3$).

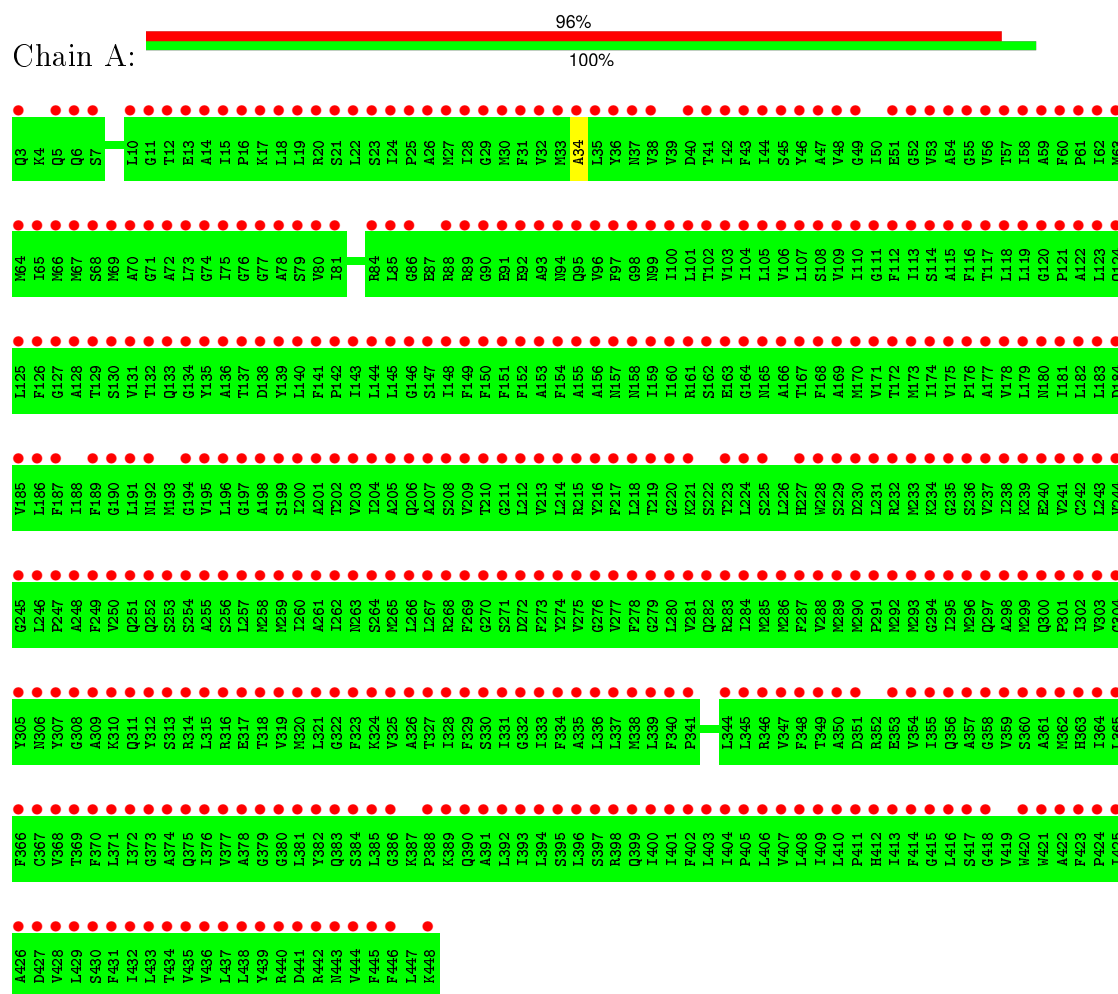


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			33	28	2	3		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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: BH2163 protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.18Å 93.89Å 102.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.70 19.98 – 3.70	Depositor EDS
% Data completeness (in resolution range)	95.0 (20.00-3.70) 95.3 (19.98-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 3.71Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.290 , 0.300 0.419 , 0.456	Depositor DCC
R_{free} test set	443 reflections (5.08%)	DCC
Wilson B-factor (Å ²)	150.9	Xtriage
Anisotropy	0.422	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.58 , 186.5	EDS
Estimated twinning fraction	0.158 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtriage
Outliers	5 of 9168 reflections (0.055%)	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	479	wwPDB-VP
Average B, all atoms (Å ²)	204.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.38% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: RHQ

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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	446	0	0	1	0
2	A	33	0	31	6	0
All	All	479	0	31	6	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 12.

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)
2:A:501:RHQ:H211	2:A:501:RHQ:H242	1.13	1.07
2:A:501:RHQ:C21	2:A:501:RHQ:H242	2.03	0.82
2:A:501:RHQ:H211	2:A:501:RHQ:C24	2.07	0.62
2:A:501:RHQ:H222	2:A:501:RHQ:H203	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ALA:CA	2:A:501:RHQ:H292	2.32	0.59
2:A:501:RHQ:C20	2:A:501:RHQ:H222	2.35	0.57

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](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 carbohydrates 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
2	RHQ	A	501	-	33,36,36	2.87	7 (21%)	40,51,51	2.14	14 (35%)

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
2	RHQ	A	501	-	-	0/15/21/21	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	RHQ	O1-C1	2.89	1.38	1.35
2	A	501	RHQ	C9-C8	3.88	1.50	1.43
2	A	501	RHQ	O2-C26	5.34	1.46	1.33
2	A	501	RHQ	C11-C12	6.29	1.52	1.40
2	A	501	RHQ	C19-C14	6.34	1.51	1.40
2	A	501	RHQ	C8-C7	7.46	1.51	1.41
2	A	501	RHQ	C2-C9	7.92	1.50	1.38

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	RHQ	C2-C9-C8	-4.93	115.91	119.57
2	A	501	RHQ	C10-C11-N1	-3.60	115.27	121.95
2	A	501	RHQ	O2-C26-O27	-2.85	118.42	123.66
2	A	501	RHQ	C21-C4-C3	-2.83	116.61	120.81
2	A	501	RHQ	C3-C2-C9	-2.75	121.11	124.27
2	A	501	RHQ	C15-C14-C19	-2.61	115.05	118.03
2	A	501	RHQ	C17-C16-C15	2.05	123.19	120.19
2	A	501	RHQ	C25-C24-N2	2.08	115.68	110.31
2	A	501	RHQ	C24-N2-C5	2.28	125.09	120.84
2	A	501	RHQ	C13-C8-C7	3.11	120.13	116.42
2	A	501	RHQ	O1-C7-C10	3.32	120.41	116.18
2	A	501	RHQ	C20-C12-C11	4.32	125.86	121.36
2	A	501	RHQ	C12-C11-N1	4.51	125.05	119.52
2	A	501	RHQ	O2-C26-C19	4.85	120.99	112.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	RHQ	6	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	446/446 (100%)	15.16	428 (95%) 0 0	116, 193, 286, 374	0

All (428) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	11	GLY	61.9
1	A	224	LEU	52.7
1	A	273	PHE	47.5
1	A	216	TYR	47.5
1	A	410	LEU	46.7
1	A	13	GLU	44.9
1	A	344	LEU	42.6
1	A	262	ILE	41.3
1	A	12	THR	40.8
1	A	233	MET	40.2
1	A	236	SER	39.7
1	A	332	GLY	38.6
1	A	49	GLY	38.1
1	A	168	PHE	36.8
1	A	443	ASN	36.7
1	A	413	ILE	35.2
1	A	204	ILE	34.6
1	A	277	VAL	34.3
1	A	390	GLN	33.7
1	A	219	THR	33.1
1	A	366	PHE	32.4
1	A	313	SER	32.0
1	A	438	LEU	31.7
1	A	345	LEU	31.7
1	A	102	THR	31.5
1	A	156	ALA	30.8
1	A	45	SER	30.6

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Mol	Chain	Res	Type	RSRZ
1	A	106	VAL	30.3
1	A	132	THR	29.8
1	A	367	CYS	29.7
1	A	349	THR	29.3
1	A	360	SER	29.3
1	A	271	SER	29.3
1	A	202	THR	28.2
1	A	357	ALA	28.0
1	A	35	LEU	27.8
1	A	164	GLY	27.8
1	A	278	PHE	27.7
1	A	264	SER	27.7
1	A	311	GLN	27.1
1	A	309	ALA	27.0
1	A	25	PRO	26.5
1	A	259	MET	26.5
1	A	350	ALA	26.1
1	A	208	SER	25.8
1	A	37	ASN	25.8
1	A	353	GLU	25.5
1	A	253	SER	25.4
1	A	147	SER	25.3
1	A	134	GLY	25.3
1	A	336	LEU	25.3
1	A	356	GLN	25.2
1	A	268	ARG	25.1
1	A	41	THR	25.1
1	A	137	THR	25.1
1	A	339	LEU	24.9
1	A	117	THR	24.8
1	A	330	SER	24.6
1	A	280	LEU	24.5
1	A	267	LEU	24.4
1	A	437	LEU	24.4
1	A	381	LEU	24.3
1	A	359	VAL	24.3
1	A	411	PRO	24.2
1	A	258	MET	24.1
1	A	421	TRP	24.0
1	A	152	PHE	23.7
1	A	284	ILE	23.6
1	A	114	SER	23.3

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Mol	Chain	Res	Type	RSRZ
1	A	163	GLU	23.3
1	A	441	ASP	23.2
1	A	250	VAL	23.2
1	A	30	MET	23.0
1	A	3	GLN	22.8
1	A	110	ILE	22.8
1	A	121	PRO	22.7
1	A	96	VAL	22.6
1	A	372	ILE	22.6
1	A	302	ILE	22.6
1	A	297	GLN	22.5
1	A	299	MET	22.5
1	A	325	VAL	22.5
1	A	252	GLN	22.4
1	A	417	SER	22.1
1	A	428	VAL	22.0
1	A	148	ILE	21.8
1	A	361	ALA	21.7
1	A	404	ILE	21.7
1	A	28	ILE	21.6
1	A	107	LEU	21.6
1	A	317	GLU	21.4
1	A	272	ASP	21.2
1	A	429	LEU	21.2
1	A	88	ARG	21.0
1	A	376	ILE	20.9
1	A	161	ARG	20.9
1	A	314	ARG	20.8
1	A	265	MET	20.8
1	A	144	LEU	20.7
1	A	118	LEU	20.7
1	A	122	ALA	20.5
1	A	225	SER	20.4
1	A	412	HIS	20.4
1	A	185	VAL	20.3
1	A	425	ILE	20.3
1	A	171	VAL	20.3
1	A	293	MET	20.2
1	A	175	VAL	20.1
1	A	261	ALA	20.0
1	A	140	LEU	19.9
1	A	337	LEU	19.9

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Mol	Chain	Res	Type	RSRZ
1	A	157	ASN	19.8
1	A	399	GLN	19.7
1	A	383	GLN	19.7
1	A	385	LEU	19.7
1	A	17	LYS	19.6
1	A	406	LEU	19.6
1	A	48	VAL	19.6
1	A	408	LEU	19.5
1	A	229	SER	19.4
1	A	85	LEU	19.4
1	A	186	LEU	19.3
1	A	91	GLU	19.2
1	A	433	LEU	19.1
1	A	254	SER	19.1
1	A	327	THR	19.0
1	A	145	LEU	19.0
1	A	207	ALA	18.9
1	A	54	ALA	18.9
1	A	141	PHE	18.9
1	A	81	ILE	18.9
1	A	94	ASN	18.7
1	A	158	ASN	18.6
1	A	315	LEU	18.6
1	A	362	MET	18.6
1	A	72	ALA	18.5
1	A	434	THR	18.5
1	A	351	ASP	18.5
1	A	282	GLN	18.4
1	A	40	ASP	18.4
1	A	246	LEU	18.4
1	A	69	MET	18.4
1	A	402	PHE	18.3
1	A	379	GLY	18.3
1	A	178	VAL	18.2
1	A	181	ILE	18.1
1	A	260	ILE	18.1
1	A	288	VAL	18.1
1	A	124	GLN	18.0
1	A	80	VAL	17.9
1	A	242	CYS	17.9
1	A	212	LEU	17.8
1	A	103	VAL	17.8

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Mol	Chain	Res	Type	RSRZ
1	A	340	PHE	17.8
1	A	210	THR	17.7
1	A	310	LYS	17.7
1	A	101	LEU	17.6
1	A	289	MET	17.6
1	A	382	TYR	17.5
1	A	401	ILE	17.5
1	A	182	LEU	17.4
1	A	266	LEU	17.2
1	A	21	SER	17.1
1	A	133	GLN	17.0
1	A	409	ILE	16.8
1	A	435	VAL	16.8
1	A	38	VAL	16.8
1	A	62	ILE	16.8
1	A	405	PRO	16.8
1	A	431	PHE	16.6
1	A	44	ILE	16.6
1	A	368	VAL	16.6
1	A	326	ALA	16.6
1	A	213	VAL	16.6
1	A	198	ALA	16.4
1	A	256	SER	16.4
1	A	281	VAL	16.3
1	A	276	GLY	16.3
1	A	20	ARG	16.2
1	A	237	VAL	16.1
1	A	279	GLY	16.1
1	A	199	SER	16.1
1	A	15	ILE	16.1
1	A	95	GLN	16.1
1	A	444	VAL	16.1
1	A	73	LEU	16.0
1	A	321	LEU	16.0
1	A	243	LEU	15.9
1	A	391	ALA	15.8
1	A	24	ILE	15.8
1	A	420	TRP	15.7
1	A	43	PHE	15.6
1	A	374	ALA	15.6
1	A	283	ARG	15.6
1	A	228	TRP	15.5

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Mol	Chain	Res	Type	RSRZ
1	A	263	ASN	15.5
1	A	369	THR	15.5
1	A	214	LEU	15.4
1	A	291	PRO	15.3
1	A	104	ILE	15.2
1	A	19	LEU	15.1
1	A	75	ILE	15.1
1	A	119	LEU	15.1
1	A	211	GLY	15.1
1	A	23	SER	15.0
1	A	55	GLY	15.0
1	A	274	TYR	15.0
1	A	257	LEU	15.0
1	A	146	GLY	14.9
1	A	397	SER	14.8
1	A	130	SER	14.7
1	A	100	ILE	14.7
1	A	194	GLY	14.6
1	A	306	ASN	14.6
1	A	396	LEU	14.6
1	A	70	ALA	14.6
1	A	329	PHE	14.6
1	A	31	PHE	14.6
1	A	14	ALA	14.5
1	A	395	SER	14.4
1	A	305	TYR	14.3
1	A	348	PHE	14.3
1	A	18	LEU	14.2
1	A	316	ARG	14.2
1	A	196	LEU	14.1
1	A	335	ALA	14.1
1	A	307	TYR	14.1
1	A	322	GLY	14.1
1	A	393	ILE	14.0
1	A	99	ASN	14.0
1	A	215	ARG	14.0
1	A	172	THR	13.9
1	A	290	MET	13.9
1	A	394	LEU	13.8
1	A	165	ASN	13.8
1	A	169	ALA	13.8
1	A	109	VAL	13.8

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Mol	Chain	Res	Type	RSRZ
1	A	292	MET	13.7
1	A	78	ALA	13.7
1	A	63	MET	13.6
1	A	333	ILE	13.5
1	A	190	GLY	13.4
1	A	131	VAL	13.3
1	A	407	VAL	13.3
1	A	142	PRO	13.3
1	A	303	VAL	13.2
1	A	86	GLY	13.0
1	A	173	MET	12.9
1	A	432	ILE	12.9
1	A	375	GLN	12.8
1	A	378	ALA	12.8
1	A	5	GLN	12.8
1	A	197	GLY	12.8
1	A	446	PHE	12.8
1	A	373	GLY	12.7
1	A	251	GLN	12.7
1	A	240	GLU	12.6
1	A	187	PHE	12.6
1	A	195	VAL	12.5
1	A	66	MET	12.5
1	A	154	PHE	12.4
1	A	138	ASP	12.3
1	A	179	LEU	12.2
1	A	60	PHE	12.2
1	A	448	LYS	12.1
1	A	71	GLY	12.1
1	A	77	GLY	12.1
1	A	177	ALA	12.0
1	A	34	ALA	11.9
1	A	7	SER	11.9
1	A	363	HIS	11.9
1	A	400	ILE	11.8
1	A	328	ILE	11.8
1	A	170	MET	11.8
1	A	76	GLY	11.7
1	A	67	MET	11.7
1	A	176	PRO	11.7
1	A	295	ILE	11.6
1	A	120	GLY	11.6

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Mol	Chain	Res	Type	RSRZ
1	A	57	THR	11.5
1	A	308	GLY	11.4
1	A	108	SER	11.4
1	A	84	ARG	11.3
1	A	318	THR	11.2
1	A	218	LEU	11.2
1	A	105	LEU	11.1
1	A	298	ALA	11.1
1	A	97	PHE	11.0
1	A	418	GLY	11.0
1	A	58	ILE	10.9
1	A	365	LEU	10.9
1	A	426	ALA	10.9
1	A	126	PHE	10.8
1	A	249	PHE	10.6
1	A	180	ASN	10.6
1	A	238	ILE	10.6
1	A	51	GLU	10.6
1	A	167	THR	10.6
1	A	209	VAL	10.5
1	A	358	GLY	10.4
1	A	153	ALA	10.3
1	A	370	PHE	10.3
1	A	430	SER	10.2
1	A	183	LEU	10.1
1	A	440	ARG	10.0
1	A	201	ALA	9.9
1	A	296	MET	9.8
1	A	245	GLY	9.8
1	A	380	GLY	9.7
1	A	203	VAL	9.7
1	A	189	PHE	9.6
1	A	33	MET	9.6
1	A	160	ILE	9.4
1	A	270	GLY	9.4
1	A	436	VAL	9.3
1	A	341	PRO	9.2
1	A	16	PRO	9.2
1	A	220	GLY	9.1
1	A	414	PHE	9.1
1	A	10	LEU	9.1
1	A	285	MET	9.0

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Mol	Chain	Res	Type	RSRZ
1	A	371	LEU	8.9
1	A	93	ALA	8.9
1	A	294	GLY	8.9
1	A	205	ALA	8.9
1	A	324	LYS	8.8
1	A	319	VAL	8.8
1	A	398	ARG	8.7
1	A	56	VAL	8.6
1	A	206	GLN	8.6
1	A	74	GLY	8.5
1	A	424	PRO	8.5
1	A	255	ALA	8.5
1	A	65	ILE	8.5
1	A	98	GLY	8.5
1	A	389	LYS	8.4
1	A	422	ALA	8.4
1	A	59	ALA	8.4
1	A	46	TYR	8.3
1	A	347	VAL	8.3
1	A	239	LYS	8.2
1	A	128	ALA	8.1
1	A	125	LEU	8.1
1	A	90	GLY	8.0
1	A	92	GLU	8.0
1	A	143	ILE	8.0
1	A	61	PRO	7.9
1	A	323	PHE	7.9
1	A	36	TYR	7.9
1	A	392	LEU	7.8
1	A	248	ALA	7.8
1	A	200	ILE	7.6
1	A	135	TYR	7.6
1	A	136	ALA	7.5
1	A	162	SER	7.5
1	A	116	PHE	7.5
1	A	191	LEU	7.5
1	A	68	SER	7.3
1	A	230	ASP	7.2
1	A	445	PHE	7.2
1	A	223	THR	7.1
1	A	79	SER	6.9
1	A	331	ILE	6.9

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Mol	Chain	Res	Type	RSRZ
1	A	32	VAL	6.8
1	A	42	ILE	6.8
1	A	384	SER	6.7
1	A	150	PHE	6.7
1	A	301	PRO	6.7
1	A	377	VAL	6.6
1	A	27	MET	6.5
1	A	139	TYR	6.4
1	A	89	ARG	6.4
1	A	300	GLN	6.3
1	A	111	GLY	6.3
1	A	64	MET	6.0
1	A	53	VAL	6.0
1	A	26	ALA	5.9
1	A	304	GLY	5.7
1	A	184	ASP	5.6
1	A	174	ILE	5.5
1	A	275	VAL	5.5
1	A	159	ILE	5.5
1	A	115	ALA	5.4
1	A	113	ILE	5.4
1	A	123	LEU	5.4
1	A	403	LEU	5.3
1	A	192	ASN	5.3
1	A	354	VAL	5.3
1	A	416	LEU	5.1
1	A	244	VAL	5.1
1	A	155	ALA	5.1
1	A	29	GLY	5.1
1	A	334	PHE	4.9
1	A	355	ILE	4.9
1	A	247	PRO	4.8
1	A	386	GLY	4.8
1	A	287	PHE	4.7
1	A	227	HIS	4.7
1	A	231	LEU	4.6
1	A	346	ARG	4.6
1	A	364	ILE	4.5
1	A	269	PHE	4.5
1	A	166	ALA	4.5
1	A	22	LEU	4.4
1	A	6	GLN	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	338	MET	4.2
1	A	442	ARG	4.2
1	A	286	MET	4.2
1	A	235	GLY	4.0
1	A	217	PHE	4.0
1	A	112	PHE	4.0
1	A	320	MET	3.9
1	A	232	ARG	3.9
1	A	129	THR	3.8
1	A	127	GLY	3.7
1	A	415	GLY	3.6
1	A	427	ASP	3.4
1	A	221	LYS	2.8
1	A	52	GLY	2.8
1	A	47	ALA	2.8
1	A	234	LYS	2.7
1	A	312	TYR	2.6
1	A	439	TYR	2.6
1	A	388	PRO	2.5
1	A	241	VAL	2.5
1	A	151	PHE	2.5
1	A	149	PHE	2.4
1	A	423	PHE	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	RHQ	A	501	33/33	0.22	1.08	-	180,300,300,300	0

6.5 Other polymers [i](#)

There are no such residues in this entry.