



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:26 PM GMT

PDB ID : 3ZFX  
Title : Crystal structure of EphB1  
Authors : Debreczeni, J.E.; Overman, R.; Truman, C.; McAlister, M.; Attwood, T.K.  
Deposited on : 2012-12-12  
Resolution : 2.50 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](mailto: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.

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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

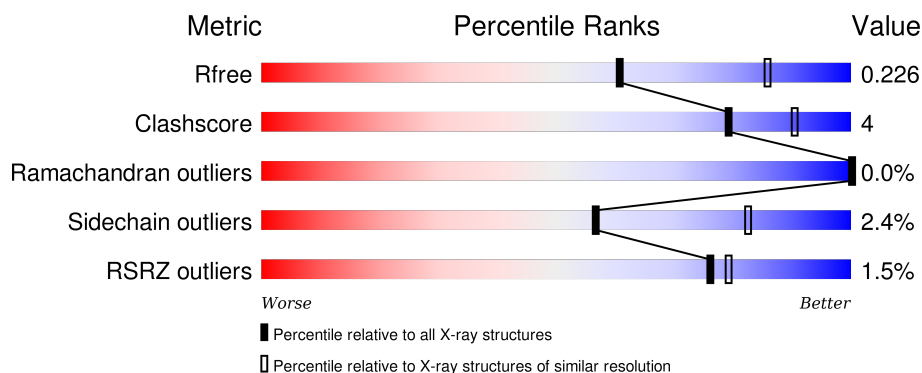
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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  $\geq 3$ , 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	298	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 77%, yellow 12%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>77%</span> <span>12%</span> <span>10%</span> </div> </div>
1	B	298	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 79%, yellow 6%, grey 15%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span></span> <span>79%</span> <span>6%</span> <span>15%</span> </div> </div>
1	C	298	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, green 76%, yellow 7%, grey 17%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>76%</span> <span>7%</span> <span>17%</span> </div> </div>
1	D	298	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 78%, yellow 10%, grey 11%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span></span> <span>78%</span> <span>10%</span> <span>11%</span> </div> </div>
1	E	298	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 78%, yellow 9%, grey 12%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>78%</span> <span>9%</span> <span>12%</span> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	298	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>79%</div><div>6%</div><div>15%</div></div></div>
1	G	298	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>78%</div><div>7%</div><div>15%</div></div></div>
1	H	298	<div><div><div></div><div></div><div></div></div><div><div></div><div>78%</div><div>10%</div><div>• 11%</div></div></div>
1	I	298	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>80%</div><div>7%</div><div>• 12%</div></div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18158 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 EPHRIN TYPE-B RECEPTOR 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	0	0
			2075	1330	350	380	15			
1	B	254	Total	C	N	O	S	0	0	0
			1961	1257	330	359	15			
1	C	248	Total	C	N	O	S	0	0	0
			1909	1223	318	353	15			
1	D	265	Total	C	N	O	S	0	0	0
			2052	1314	345	378	15			
1	E	262	Total	C	N	O	S	0	0	0
			2021	1294	339	373	15			
1	F	254	Total	C	N	O	S	0	0	0
			1946	1248	317	366	15			
1	G	253	Total	C	N	O	S	0	0	0
			1974	1261	332	366	15			
1	H	266	Total	C	N	O	S	0	0	0
			2051	1316	344	376	15			
1	I	263	Total	C	N	O	S	0	0	0
			2030	1300	343	372	15			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	599	GLY	-	EXPRESSION TAG	UNP P54762
A	600	SER	-	EXPRESSION TAG	UNP P54762
A	601	SER	-	EXPRESSION TAG	UNP P54762
B	599	GLY	-	EXPRESSION TAG	UNP P54762
B	600	SER	-	EXPRESSION TAG	UNP P54762
B	601	SER	-	EXPRESSION TAG	UNP P54762
C	599	GLY	-	EXPRESSION TAG	UNP P54762
C	600	SER	-	EXPRESSION TAG	UNP P54762
C	601	SER	-	EXPRESSION TAG	UNP P54762
D	599	GLY	-	EXPRESSION TAG	UNP P54762
D	600	SER	-	EXPRESSION TAG	UNP P54762

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Chain	Residue	Modelled	Actual	Comment	Reference
D	601	SER	-	EXPRESSION TAG	UNP P54762
E	599	GLY	-	EXPRESSION TAG	UNP P54762
E	600	SER	-	EXPRESSION TAG	UNP P54762
E	601	SER	-	EXPRESSION TAG	UNP P54762
F	599	GLY	-	EXPRESSION TAG	UNP P54762
F	600	SER	-	EXPRESSION TAG	UNP P54762
F	601	SER	-	EXPRESSION TAG	UNP P54762
G	599	GLY	-	EXPRESSION TAG	UNP P54762
G	600	SER	-	EXPRESSION TAG	UNP P54762
G	601	SER	-	EXPRESSION TAG	UNP P54762
H	599	GLY	-	EXPRESSION TAG	UNP P54762
H	600	SER	-	EXPRESSION TAG	UNP P54762
H	601	SER	-	EXPRESSION TAG	UNP P54762
I	599	GLY	-	EXPRESSION TAG	UNP P54762
I	600	SER	-	EXPRESSION TAG	UNP P54762
I	601	SER	-	EXPRESSION TAG	UNP P54762

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

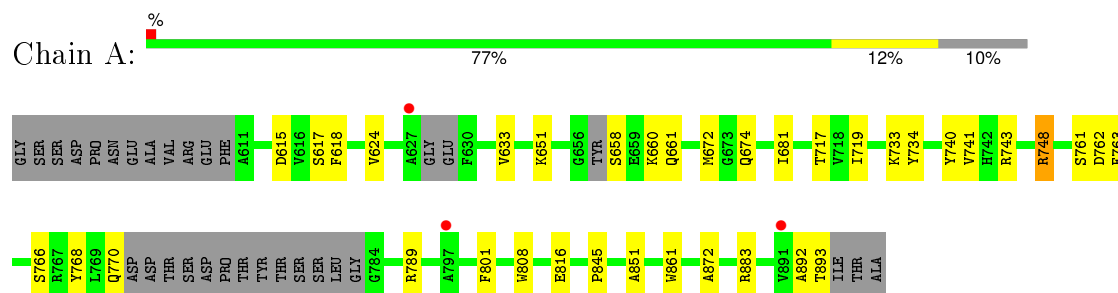
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	52	Total 52	O 52	0	0
3	B	7	Total 7	O 7	0	0
3	C	1	Total 1	O 1	0	0
3	D	39	Total 39	O 39	0	0
3	E	3	Total 3	O 3	0	0
3	F	4	Total 4	O 4	0	0
3	G	5	Total 5	O 5	0	0
3	H	17	Total 17	O 17	0	0
3	I	6	Total 6	O 6	0	0

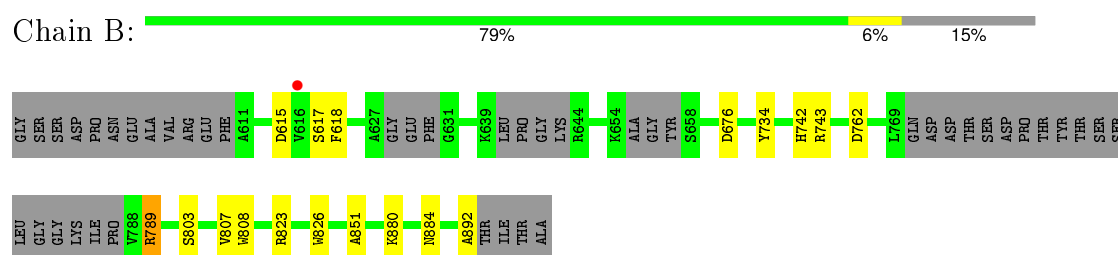
### 3 Residue-property plots [i](#)

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 ( $RSRZ > 2$ ). 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.

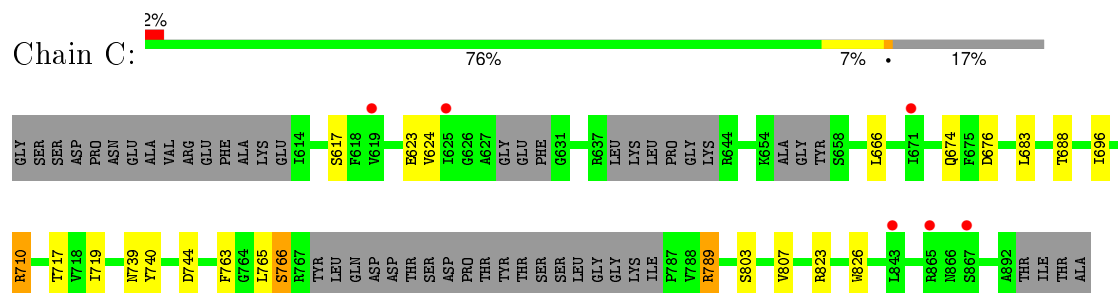
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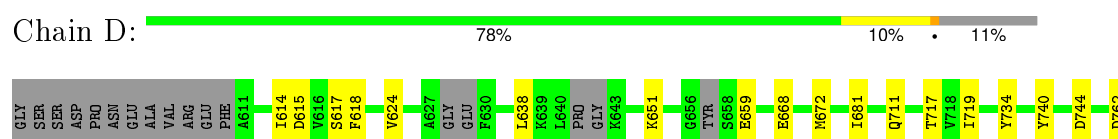
#### • Molecule 1: EPHRIN TYPE-B RECEPTOR 1

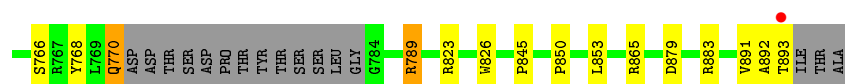


#### • Molecule 1: EPHRIN TYPE-B RECEPTOR 1

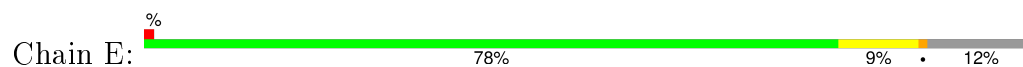


#### • Molecule 1: EPHRIN TYPE-B RECEPTOR 1

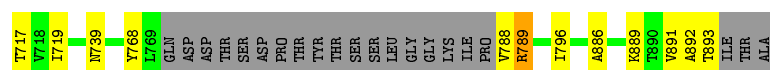
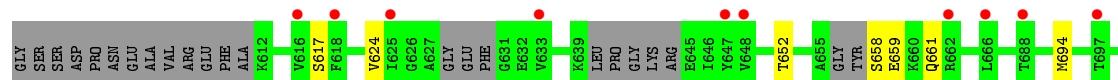
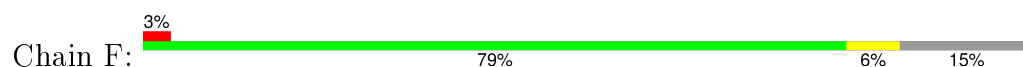




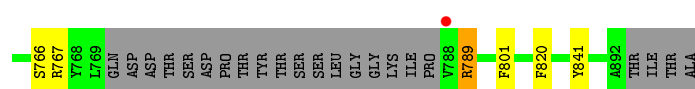
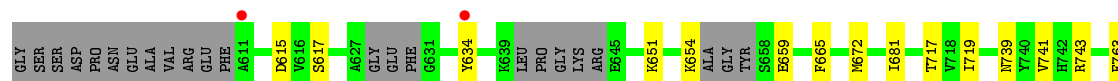
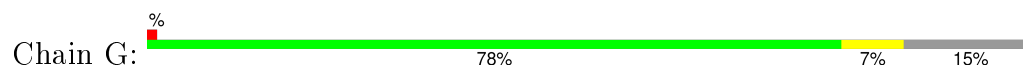
• Molecule 1: EPHRIN TYPE-B RECEPTOR 1



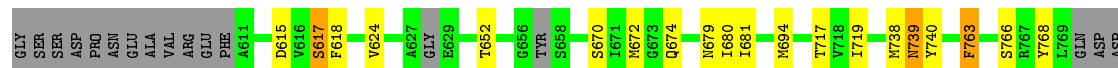
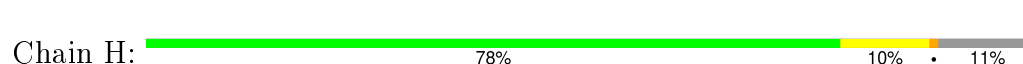
• Molecule 1: EPHRIN TYPE-B RECEPTOR 1



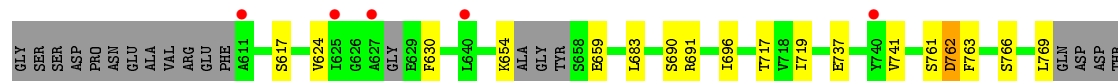
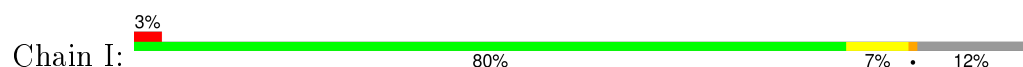
• Molecule 1: EPHRIN TYPE-B RECEPTOR 1



• Molecule 1: EPHRIN TYPE-B RECEPTOR 1



• Molecule 1: EPHRIN TYPE-B RECEPTOR 1







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	195.98 Å 195.98 Å 60.24 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.50 84.86 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (15.00-2.50) 100.0 (84.86-2.50)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.93 (at 2.51 Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.188 , 0.217 0.203 , 0.226	Depositor DCC
$R_{free}$ test set	4548 reflections (5.38%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.7	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 43.2	EDS
Estimated twinning fraction	0.031 for H, K, L 0.030 for -K, -H, -L 0.432 for -H, -K, L 0.507 for K, H, -L 0.000 for -h,-k,l 0.000 for h,-h-k,-l 0.097 for -k,-h,-l	Xtriage
Reported twinning fraction	0.031 for H, K, L 0.030 for -K, -H, -L 0.432 for -H, -K, L 0.507 for K, H, -L	Depositor
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 89479 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	18158	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.38 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.0458e-04. The detected translational NCS is most likely*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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.

*also responsible for the elevated intensity ratio.*

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.70	2/2116 (0.1%)	0.95	6/2863 (0.2%)
1	B	0.77	4/1998 (0.2%)	0.74	2/2705 (0.1%)
1	C	0.50	0/1946	0.93	5/2638 (0.2%)
1	D	0.65	0/2090	0.86	4/2828 (0.1%)
1	E	0.75	8/2059 (0.4%)	0.74	3/2790 (0.1%)
1	F	0.49	0/1983	0.69	2/2692 (0.1%)
1	G	0.86	12/2011 (0.6%)	0.81	3/2723 (0.1%)
1	H	0.81	8/2092 (0.4%)	0.84	3/2833 (0.1%)
1	I	0.65	4/2070 (0.2%)	0.75	3/2804 (0.1%)
All	All	0.70	38/18365 (0.2%)	0.82	31/24876 (0.1%)

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	C	0	1

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	734	TYR	CE1-CZ	-14.83	1.19	1.38
1	E	634	TYR	CE1-CZ	-12.59	1.22	1.38
1	I	841	TYR	CE1-CZ	-12.56	1.22	1.38
1	B	734	TYR	CG-CD2	-11.71	1.24	1.39
1	G	841	TYR	CE1-CZ	-11.59	1.23	1.38
1	G	634	TYR	CE1-CZ	-11.45	1.23	1.38
1	B	734	TYR	CE2-CZ	-11.36	1.23	1.38
1	B	734	TYR	CG-CD1	-11.24	1.24	1.39
1	E	634	TYR	CG-CD2	-10.58	1.25	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	748	ARG	CZ-NH2	-10.53	1.19	1.33
1	E	634	TYR	CG-CD1	-10.40	1.25	1.39
1	G	841	TYR	CG-CD2	-10.14	1.25	1.39
1	G	634	TYR	CG-CD1	-10.00	1.26	1.39
1	I	841	TYR	CG-CD2	-9.70	1.26	1.39
1	I	841	TYR	CG-CD1	-9.63	1.26	1.39
1	H	763	PHE	CG-CD2	-9.60	1.24	1.38
1	G	841	TYR	CG-CD1	-9.46	1.26	1.39
1	H	763	PHE	CG-CD1	-9.31	1.24	1.38
1	G	634	TYR	CG-CD2	-9.26	1.27	1.39
1	E	634	TYR	CE2-CZ	-9.00	1.26	1.38
1	G	820	PHE	CG-CD2	-8.65	1.25	1.38
1	H	820	PHE	CG-CD1	-8.58	1.25	1.38
1	G	841	TYR	CE2-CZ	-8.44	1.27	1.38
1	G	634	TYR	CE2-CZ	-8.21	1.27	1.38
1	I	841	TYR	CE2-CZ	-8.19	1.27	1.38
1	G	820	PHE	CG-CD1	-8.18	1.26	1.38
1	E	763	PHE	CG-CD2	-7.98	1.26	1.38
1	H	820	PHE	CG-CD2	-7.92	1.26	1.38
1	E	763	PHE	CG-CD1	-7.81	1.27	1.38
1	A	748	ARG	CZ-NH1	-7.37	1.23	1.33
1	H	763	PHE	CE2-CZ	-6.19	1.25	1.37
1	H	763	PHE	CE1-CZ	-6.06	1.25	1.37
1	G	820	PHE	CE1-CZ	-5.70	1.26	1.37
1	H	820	PHE	CE2-CZ	-5.67	1.26	1.37
1	E	763	PHE	CE1-CZ	-5.43	1.27	1.37
1	H	820	PHE	CE1-CZ	-5.36	1.27	1.37
1	G	820	PHE	CE2-CZ	-5.21	1.27	1.37
1	E	763	PHE	CE2-CZ	-5.18	1.27	1.37

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	710	ARG	NE-CZ-NH2	-24.68	107.96	120.30
1	A	748	ARG	NE-CZ-NH1	19.30	129.95	120.30
1	C	710	ARG	NE-CZ-NH1	17.56	129.08	120.30
1	D	789	ARG	NE-CZ-NH2	-15.96	112.32	120.30
1	I	789	ARG	NE-CZ-NH2	-15.64	112.48	120.30
1	I	789	ARG	NE-CZ-NH1	14.28	127.44	120.30
1	D	789	ARG	NE-CZ-NH1	14.22	127.41	120.30
1	A	789	ARG	NE-CZ-NH1	13.47	127.04	120.30
1	E	789	ARG	NE-CZ-NH2	-13.02	113.79	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	789	ARG	NE-CZ-NH2	-12.97	113.82	120.30
1	C	710	ARG	CD-NE-CZ	12.71	141.40	123.60
1	H	789	ARG	NE-CZ-NH2	-12.66	113.97	120.30
1	E	789	ARG	NE-CZ-NH1	12.60	126.60	120.30
1	H	789	ARG	NE-CZ-NH1	12.54	126.57	120.30
1	G	789	ARG	NE-CZ-NH1	11.95	126.28	120.30
1	F	789	ARG	NE-CZ-NH2	-11.95	114.33	120.30
1	G	789	ARG	NE-CZ-NH2	-11.60	114.50	120.30
1	A	748	ARG	NH1-CZ-NH2	-11.51	106.75	119.40
1	F	789	ARG	NE-CZ-NH1	11.29	125.95	120.30
1	C	789	ARG	NE-CZ-NH2	-11.00	114.80	120.30
1	C	789	ARG	NE-CZ-NH1	10.98	125.79	120.30
1	B	789	ARG	NE-CZ-NH1	10.71	125.65	120.30
1	B	789	ARG	NE-CZ-NH2	-10.70	114.95	120.30
1	A	748	ARG	CG-CD-NE	-7.88	95.25	111.80
1	A	789	ARG	CD-NE-CZ	6.53	132.75	123.60
1	D	789	ARG	CD-NE-CZ	6.36	132.50	123.60
1	D	744	ASP	CB-CG-OD1	6.20	123.88	118.30
1	I	789	ARG	CD-NE-CZ	6.17	132.23	123.60
1	H	789	ARG	CD-NE-CZ	6.01	132.01	123.60
1	G	789	ARG	CD-NE-CZ	5.18	130.85	123.60
1	E	789	ARG	CD-NE-CZ	5.14	130.79	123.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	710	ARG	Sidechain

## 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	2075	0	2028	21	1
1	B	1961	0	1896	7	1
1	C	1909	0	1831	11	0
1	D	2052	0	1999	15	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2021	0	1953	15	1
1	F	1946	0	1850	9	1
1	G	1974	0	1910	13	0
1	H	2051	0	1993	19	0
1	I	2030	0	1969	18	0
2	A	5	0	0	0	0
3	A	52	0	0	4	0
3	B	7	0	0	0	0
3	C	1	0	0	0	0
3	D	39	0	0	0	0
3	E	3	0	0	0	0
3	F	4	0	0	0	0
3	G	5	0	0	0	0
3	H	17	0	0	0	0
3	I	6	0	0	0	0
All	All	18158	0	17429	124	3

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 4.

All (124) 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:I:741:VAL:HG23	1:I:769:LEU:HD11	1.49	0.94
1:D:651:LYS:NZ	1:D:668:GLU:OE1	2.09	0.84
1:G:741:VAL:HG12	1:G:743:ARG:HG2	1.60	0.83
1:A:816:GLU:OE2	3:A:2026:HOH:O	2.03	0.75
1:I:741:VAL:CG2	1:I:769:LEU:HD11	2.17	0.75
1:I:741:VAL:HG23	1:I:769:LEU:CD1	2.19	0.71
1:F:658:SER:OG	1:F:661:GLN:HG3	1.94	0.68
1:I:741:VAL:HG21	1:I:769:LEU:HD21	1.79	0.65
1:A:658:SER:OG	1:A:661:GLN:HG3	1.96	0.65
1:G:743:ARG:HD2	1:G:801:PHE:CD2	2.32	0.64
1:E:741:VAL:CG2	1:E:769:LEU:HD21	2.28	0.63
1:H:670:SER:O	1:H:674:GLN:NE2	2.32	0.63
1:D:614:ILE:HD13	1:D:638:LEU:HD11	1.82	0.62
1:H:851:ALA:HA	1:H:892:ALA:HB2	1.82	0.60
1:H:823:ARG:HD3	1:H:826:TRP:O	2.03	0.59
1:I:741:VAL:CG2	1:I:769:LEU:HD21	2.33	0.58
1:H:652:THR:HG22	1:H:694:MET:HG2	1.86	0.58
1:B:851:ALA:HA	1:B:892:ALA:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:744:ASP:HB2	1:C:765:LEU:HD22	1.86	0.58
1:E:741:VAL:HG21	1:E:769:LEU:HD21	1.86	0.56
1:H:717:THR:OG1	1:H:719:ILE:HG22	2.05	0.56
1:E:823:ARG:NH1	1:E:826:TRP:O	2.39	0.55
1:A:845:PRO:HG2	1:A:893:THR:CB	2.37	0.54
1:C:624:VAL:O	1:C:624:VAL:HG13	2.07	0.54
1:A:851:ALA:HA	1:A:892:ALA:HB2	1.90	0.54
1:I:763:PHE:O	1:I:766:SER:HB2	2.08	0.53
1:E:789:ARG:CZ	1:E:823:ARG:NH2	2.72	0.53
1:G:672:MET:SD	1:G:681:ILE:HG23	2.50	0.52
1:A:717:THR:OG1	1:A:719:ILE:HG22	2.09	0.52
1:H:763:PHE:O	1:H:766:SER:HB2	2.09	0.52
1:A:672:MET:SD	1:A:681:ILE:HG23	2.49	0.52
1:F:624:VAL:O	1:F:624:VAL:HG13	2.10	0.52
1:G:741:VAL:CG1	1:G:743:ARG:HG2	2.38	0.52
1:D:615:ASP:HB3	1:D:618:PHE:CE2	2.45	0.52
1:F:652:THR:HG22	1:F:694:MET:HG2	1.92	0.51
1:E:763:PHE:O	1:E:766:SER:HB2	2.11	0.50
1:D:624:VAL:HG13	1:D:624:VAL:O	2.11	0.50
1:A:761:SER:OG	1:A:762:ASP:N	2.44	0.50
1:D:717:THR:OG1	1:D:719:ILE:HG22	2.12	0.50
1:D:823:ARG:NH1	1:D:826:TRP:O	2.39	0.50
1:I:624:VAL:O	1:I:624:VAL:HG13	2.12	0.50
1:G:743:ARG:HD2	1:G:801:PHE:CG	2.47	0.49
1:C:666:LEU:HD21	1:C:688:THR:HG22	1.95	0.49
1:I:741:VAL:HG23	1:I:769:LEU:CG	2.42	0.49
1:A:741:VAL:HG12	1:A:743:ARG:HG2	1.94	0.49
1:H:740:TYR:CE1	1:H:768:TYR:HB2	2.48	0.49
1:E:814:MET:HE1	1:E:856:LEU:HB3	1.95	0.49
1:C:823:ARG:HD3	1:C:826:TRP:O	2.12	0.48
1:A:748:ARG:HB3	3:A:2014:HOH:O	2.12	0.48
1:G:743:ARG:NH2	1:G:767:ARG:HG3	2.28	0.48
1:H:679:ASN:O	1:H:680:ILE:HD13	2.13	0.48
1:B:615:ASP:HB3	1:B:618:PHE:CE2	2.49	0.48
1:I:761:SER:OG	1:I:762:ASP:N	2.47	0.48
1:D:850:PRO:HG2	1:D:853:LEU:HD12	1.95	0.48
1:G:743:ARG:HD3	1:G:801:PHE:CB	2.44	0.47
1:F:891:VAL:HG12	1:F:892:ALA:N	2.29	0.47
1:D:672:MET:SD	1:D:681:ILE:HG23	2.54	0.47
1:E:803:SER:O	1:E:807:VAL:HG23	2.14	0.47
1:A:633:VAL:HG22	1:A:651:LYS:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:733:LYS:HD2	1:A:872:ALA:HA	1.97	0.47
1:A:740:TYR:CE2	1:A:768:TYR:HB2	2.50	0.47
1:D:768:TYR:CE2	1:D:770:GLN:HB3	2.51	0.46
1:E:761:SER:OG	1:E:762:ASP:N	2.48	0.46
1:C:717:THR:OG1	1:C:719:ILE:HG22	2.15	0.46
1:E:717:THR:OG1	1:E:719:ILE:HG22	2.15	0.46
1:H:615:ASP:OD1	1:H:617:SER:OG	2.32	0.46
1:B:803:SER:O	1:B:807:VAL:HG23	2.16	0.46
1:D:845:PRO:HG2	1:D:893:THR:CB	2.45	0.46
1:A:748:ARG:CB	3:A:2014:HOH:O	2.64	0.46
1:A:674:GLN:OE1	1:A:740:TYR:OH	2.30	0.46
1:I:683:LEU:HD12	1:I:696:ILE:O	2.15	0.46
1:D:891:VAL:HG12	1:D:892:ALA:N	2.31	0.45
1:G:743:ARG:CD	1:G:801:PHE:CG	3.00	0.45
1:C:666:LEU:CD2	1:C:688:THR:HG22	2.47	0.45
1:D:740:TYR:CZ	1:D:768:TYR:CD1	3.04	0.45
1:A:883:ARG:HH11	1:B:676:ASP:HB2	1.81	0.45
1:A:615:ASP:HB3	1:A:618:PHE:CE2	2.52	0.45
1:I:803:SER:O	1:I:807:VAL:HG23	2.16	0.44
1:G:743:ARG:HH11	1:G:801:PHE:HB2	1.82	0.44
1:A:743:ARG:HD3	1:A:801:PHE:CG	2.53	0.44
1:A:763:PHE:HA	3:A:2023:HOH:O	2.17	0.44
1:H:850:PRO:HG2	1:H:853:LEU:HD12	1.99	0.44
1:G:763:PHE:O	1:G:766:SER:HB2	2.18	0.44
1:F:717:THR:OG1	1:F:719:ILE:HG22	2.18	0.44
1:H:811:GLY:O	1:H:814:MET:HB2	2.18	0.44
1:F:889:LYS:HD3	1:F:889:LYS:N	2.33	0.43
1:C:803:SER:O	1:C:807:VAL:HG23	2.17	0.43
1:I:814:MET:CE	1:I:856:LEU:HD23	2.49	0.43
1:E:845:PRO:HG2	1:E:893:THR:CB	2.48	0.43
1:H:672:MET:SD	1:H:681:ILE:HG23	2.58	0.43
1:I:814:MET:HE1	1:I:856:LEU:HB3	2.00	0.43
1:G:651:LYS:HD3	1:G:665:PHE:HE1	1.84	0.43
1:D:768:TYR:CZ	1:D:770:GLN:HB3	2.54	0.43
1:E:683:LEU:HD12	1:E:696:ILE:O	2.19	0.43
1:H:738:MET:O	1:H:739:ASN:HB2	2.20	0.42
1:E:789:ARG:HG2	1:E:790:TRP:CE3	2.55	0.42
1:E:841:TYR:HE1	1:I:691:ARG:O	2.03	0.42
1:D:879:ASP:O	1:D:883:ARG:HG2	2.19	0.42
1:I:717:THR:OG1	1:I:719:ILE:HG22	2.20	0.42
1:C:763:PHE:O	1:C:766:SER:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:659:GLU:C	1:F:659:GLU:CD	2.79	0.42
1:B:808:TRP:C	1:B:808:TRP:CD1	2.93	0.42
1:H:841:TYR:O	1:H:842:ARG:HD3	2.20	0.41
1:H:615:ASP:HB3	1:H:618:PHE:CE2	2.54	0.41
1:C:676:ASP:HB3	1:H:739:ASN:HD21	1.85	0.41
1:B:742:HIS:O	1:B:743:ARG:HB2	2.21	0.41
1:G:615:ASP:OD1	1:G:615:ASP:C	2.59	0.41
1:H:674:GLN:OE1	1:H:740:TYR:OH	2.36	0.41
1:D:740:TYR:CE1	1:D:768:TYR:HB2	2.55	0.41
1:F:886:ALA:HA	1:F:889:LYS:HG2	2.01	0.41
1:H:615:ASP:C	1:H:615:ASP:OD1	2.59	0.41
1:B:823:ARG:HD3	1:B:826:TRP:O	2.19	0.41
1:F:788:VAL:HG13	1:F:796:ILE:CD1	2.51	0.41
1:A:808:TRP:CE3	1:A:861:TRP:HA	2.56	0.41
1:H:624:VAL:HG13	1:H:624:VAL:O	2.19	0.41
1:E:841:TYR:CD1	1:I:690:SER:HB2	2.56	0.40
1:A:763:PHE:O	1:A:766:SER:HB2	2.22	0.40
1:I:630:PHE:HB2	1:I:654:LYS:NZ	2.37	0.40
1:I:630:PHE:HB2	1:I:654:LYS:HZ2	1.86	0.40
1:C:674:GLN:OE1	1:C:740:TYR:OH	2.32	0.40
1:G:717:THR:OG1	1:G:719:ILE:HG22	2.22	0.40
1:A:624:VAL:HG13	1:A:624:VAL:O	2.21	0.40
1:C:683:LEU:HD12	1:C:696:ILE:O	2.22	0.40
1:E:741:VAL:HG23	1:E:769:LEU:HD21	2.02	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:734:TYR:OH	1:B:884:ASN:ND2[1_556]	1.93	0.27
1:D:734:TYR:OH	1:E:884:ASN:OD1[3_554]	2.09	0.11
1:D:865:ARG:NH1	1:F:768:TYR:OH[1_554]	2.18	0.02

## 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	259/298 (87%)	248 (96%)	11 (4%)	0	100	100
1	B	244/298 (82%)	237 (97%)	7 (3%)	0	100	100
1	C	238/298 (80%)	230 (97%)	8 (3%)	0	100	100
1	D	255/298 (86%)	245 (96%)	10 (4%)	0	100	100
1	E	252/298 (85%)	240 (95%)	11 (4%)	1 (0%)	39	61
1	F	244/298 (82%)	237 (97%)	7 (3%)	0	100	100
1	G	243/298 (82%)	237 (98%)	6 (2%)	0	100	100
1	H	258/298 (87%)	251 (97%)	7 (3%)	0	100	100
1	I	255/298 (86%)	246 (96%)	9 (4%)	0	100	100
All	All	2248/2682 (84%)	2171 (97%)	76 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	788	VAL

### 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	214/256 (84%)	211 (99%)	3 (1%)	74	91
1	B	200/256 (78%)	196 (98%)	4 (2%)	63	86
1	C	195/256 (76%)	190 (97%)	5 (3%)	54	81
1	D	211/256 (82%)	204 (97%)	7 (3%)	45	73
1	E	207/256 (81%)	199 (96%)	8 (4%)	39	66
1	F	198/256 (77%)	194 (98%)	4 (2%)	63	86
1	G	205/256 (80%)	200 (98%)	5 (2%)	57	82
1	H	210/256 (82%)	206 (98%)	4 (2%)	65	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	I	209/256 (82%)	204 (98%)	5 (2%)	57 82
All	All	1849/2304 (80%)	1804 (98%)	45 (2%)	57 82

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	617	SER
1	A	660	LYS
1	A	770	GLN
1	B	617	SER
1	B	762	ASP
1	B	789	ARG
1	B	880	LYS
1	C	617	SER
1	C	623	GLU
1	C	739	ASN
1	C	766	SER
1	C	789	ARG
1	D	617	SER
1	D	659	GLU
1	D	711	GLN
1	D	762	ASP
1	D	766	SER
1	D	770	GLN
1	D	789	ARG
1	E	612	LYS
1	E	615	ASP
1	E	617	SER
1	E	640	LEU
1	E	651	LYS
1	E	739	ASN
1	E	762	ASP
1	E	789	ARG
1	F	617	SER
1	F	739	ASN
1	F	789	ARG
1	F	893	THR
1	G	617	SER
1	G	654	LYS
1	G	659	GLU
1	G	739	ASN
1	G	789	ARG

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Mol	Chain	Res	Type
1	H	617	SER
1	H	739	ASN
1	H	789	ARG
1	H	883	ARG
1	I	617	SER
1	I	659	GLU
1	I	737	GLU
1	I	762	ASP
1	I	789	ARG

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

Mol	Chain	Res	Type
1	C	862	GLN
1	F	862	GLN
1	G	862	GLN
1	H	862	GLN

### 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	SO4	A	1890	-	4,4,4	1.00	0	6,6,6	0.23	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
2	SO4	A	1890	-	-	0/0/0/0	0/0/0/0

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.

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	267/298 (89%)	0.08	3 (1%) 82 84	17, 26, 40, 44	0
1	B	254/298 (85%)	0.05	1 (0%) 93 93	28, 35, 46, 49	0
1	C	248/298 (83%)	0.16	6 (2%) 62 66	35, 41, 48, 52	0
1	D	265/298 (88%)	-0.08	1 (0%) 93 93	14, 23, 33, 42	0
1	E	262/298 (87%)	0.08	3 (1%) 82 84	28, 36, 47, 53	0
1	F	254/298 (85%)	0.27	10 (3%) 43 48	34, 40, 52, 58	0
1	G	253/298 (84%)	0.04	3 (1%) 81 83	26, 34, 47, 52	0
1	H	266/298 (89%)	-0.13	0 100 100	14, 24, 34, 42	0
1	I	263/298 (88%)	0.41	8 (3%) 54 59	37, 43, 51, 56	0
All	All	2332/2682 (86%)	0.10	35 (1%) 76 79	14, 35, 48, 58	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	611	ALA	4.0
1	F	647	TYR	3.8
1	E	893	THR	3.5
1	I	784	GLY	3.4
1	I	625	ILE	3.4
1	F	625	ILE	3.0
1	C	619	VAL	2.9
1	I	872	ALA	2.9
1	F	688	THR	2.8
1	F	666	LEU	2.8
1	E	621	ILE	2.8
1	I	788	VAL	2.7
1	A	797	ALA	2.6
1	C	867	SER	2.5
1	A	891	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	826	TRP	2.5
1	C	865	ARG	2.4
1	F	648	VAL	2.4
1	C	625	ILE	2.3
1	I	627	ALA	2.3
1	D	893	THR	2.3
1	F	662	ARG	2.3
1	B	616	VAL	2.2
1	F	697	THR	2.2
1	G	611	ALA	2.2
1	F	618	PHE	2.2
1	A	627	ALA	2.1
1	C	843	LEU	2.1
1	F	616	VAL	2.1
1	F	633	VAL	2.1
1	G	788	VAL	2.1
1	C	671	ILE	2.1
1	G	634	TYR	2.1
1	I	740	TYR	2.0
1	I	640	LEU	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 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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
2	SO4	A	1890	5/5	0.96	0.10	-	25,28,32,38	0



## 6.5 Other polymers [i](#)

There are no such residues in this entry.