



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:22 PM UTC

PDB ID : 2CGO / pdb_00002cgo
Title : FACTOR INHIBITING HIF-1 ALPHA with fumarate
Authors : McDonough, M.A.; Clifton, I.J.; Schofield, C.J.
Deposited on : 2006-03-09
Resolution : 2.30 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

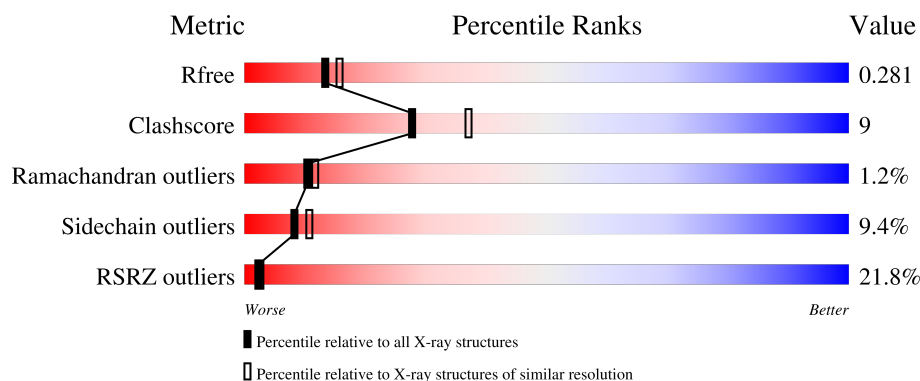
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	349	21% 73% 18% 6% ...

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2932 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.

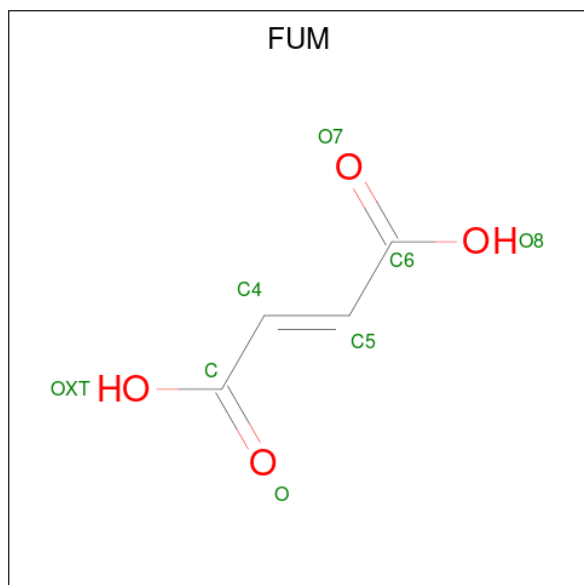
- Molecule 1 is a protein called HYPOXIA-INDUCIBLE FACTOR 1 ALPHA INHIBITOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	0	0
			2777	1779	473	514	11			

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		

- Molecule 3 is FUMARIC ACID (CCD ID: FUM) (formula: C₄H₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	4	4		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	1
			10	8	2		
4	A	1	Total	O	S	0	0
			5	4	1		

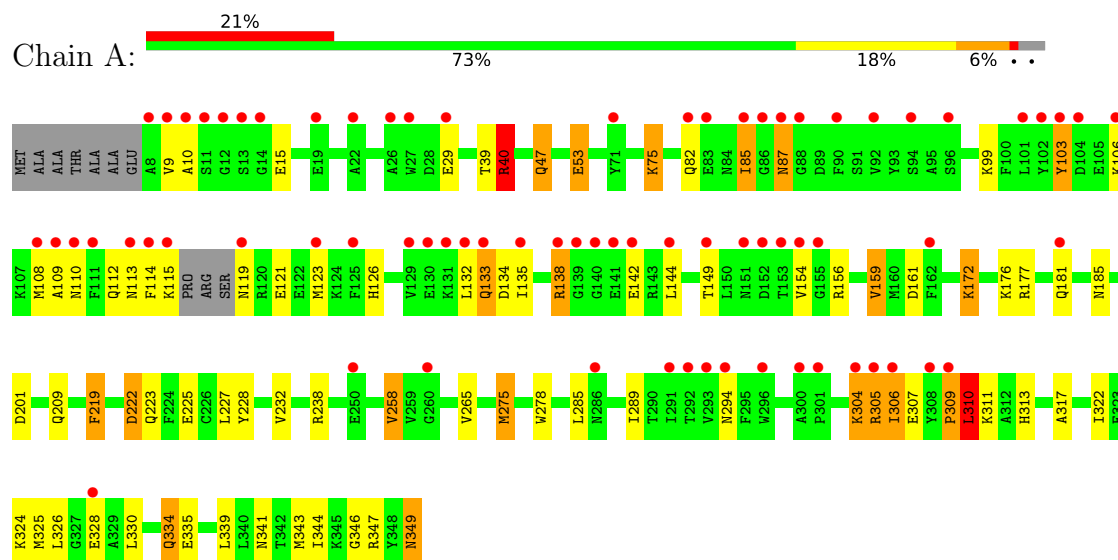
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	121	Total	O	0	0
			121	121		

3 Residue-property plots [i](#)

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: HYPOXIA-INDUCIBLE FACTOR 1 ALPHA INHIBITOR



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	86.66Å 86.66Å 147.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.74 – 2.30 74.70 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (74.74-2.30) 99.6 (74.70-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.187 , 0.237 0.247 , 0.281	Depositor DCC
R_{free} test set	2532 reflections (9.83%)	wwPDB-VP
Wilson B-factor (Å ²)	50.9	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2932	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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: FUM, FE, 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	1.46	14/2857 (0.5%)	1.21	5/3877 (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	A	0	1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	347	ARG	N-CA	7.53	1.54	1.46
1	A	265	VAL	CA-CB	7.25	1.62	1.54
1	A	222	ASP	C-O	-7.12	1.13	1.24
1	A	228	TYR	C-O	6.84	1.27	1.23
1	A	103	TYR	C-O	-6.77	1.16	1.24
1	A	344	ILE	CA-CB	6.16	1.62	1.54
1	A	225	GLU	N-CA	5.77	1.53	1.46
1	A	238	ARG	CZ-NH1	5.73	1.40	1.32
1	A	328	GLU	C-O	-5.60	1.17	1.24
1	A	219	PHE	CA-C	5.37	1.57	1.52
1	A	209	GLN	C-O	5.29	1.30	1.23
1	A	201	ASP	CG-OD2	5.21	1.35	1.25
1	A	317	ALA	CA-CB	5.21	1.61	1.53
1	A	40	ARG	CG-CD	5.08	1.67	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	VAL	N-CA-C	-6.35	104.30	110.72
1	A	341	ASN	N-CA-C	6.11	117.60	111.07
1	A	40	ARG	N-CA-CB	-5.63	100.80	110.72
1	A	343	MET	N-CA-C	5.22	116.97	111.28
1	A	47	GLN	N-CA-C	-5.01	106.43	112.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	304	LYS	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	2777	0	2660	49	0
2	A	1	0	0	0	0
3	A	8	0	1	0	0
4	A	25	0	0	0	0
5	A	121	0	0	5	0
All	All	2932	0	2661	49	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 9.

All (49) 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:119:ASN:HA	5:A:2045:HOH:O	1.82	0.78
1:A:176:LYS:NZ	5:A:2057:HOH:O	2.15	0.77
1:A:334:GLN:HE21	1:A:334:GLN:HA	1.53	0.71
1:A:309:PRO:O	1:A:310:LEU:HB2	1.91	0.70
1:A:85:ILE:CD1	1:A:85:ILE:O	2.43	0.66
1:A:112:GLN:O	1:A:114:PHE:N	2.31	0.64
1:A:9:VAL:HG12	1:A:40:ARG:HD2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:GLN:HE21	1:A:133:GLN:HA	1.64	0.63
1:A:132:LEU:HD23	1:A:144:LEU:HD12	1.80	0.61
1:A:306:ILE:HD13	1:A:306:ILE:N	2.16	0.60
1:A:322:ILE:HA	1:A:325:MET:HE2	1.84	0.58
1:A:85:ILE:O	1:A:85:ILE:HD13	2.05	0.56
1:A:305:ARG:HB3	1:A:306:ILE:HD13	1.88	0.55
1:A:53:GLU:HG3	1:A:177:ARG:HH22	1.72	0.54
1:A:219:PHE:HB2	1:A:278:TRP:HB2	1.89	0.53
1:A:334:GLN:HE21	1:A:334:GLN:CA	2.20	0.53
1:A:87:ASN:N	1:A:87:ASN:OD1	2.43	0.52
1:A:85:ILE:O	1:A:85:ILE:HD12	2.08	0.52
1:A:275:MET:HE1	5:A:2027:HOH:O	2.10	0.51
1:A:223:GLN:NE2	1:A:258:VAL:HG22	2.25	0.51
1:A:346:GLY:H	1:A:349:ASN:HD21	1.59	0.51
1:A:223:GLN:HE21	1:A:258:VAL:HG23	1.77	0.50
1:A:115:LYS:N	5:A:2044:HOH:O	2.38	0.49
1:A:223:GLN:NE2	1:A:258:VAL:CG2	2.76	0.49
1:A:75:LYS:NZ	1:A:161:ASP:OD1	2.46	0.48
1:A:330:LEU:HD13	1:A:335:GLU:HB3	1.96	0.47
1:A:326:LEU:HD11	1:A:339:LEU:HD22	1.97	0.47
1:A:10:ALA:HA	1:A:39:THR:O	2.15	0.47
1:A:115:LYS:HB2	5:A:2044:HOH:O	2.14	0.47
1:A:306:ILE:HD13	1:A:306:ILE:H	1.80	0.47
1:A:134:ASP:OD2	1:A:138:ARG:NH1	2.48	0.46
1:A:135:ILE:HD13	1:A:142:GLU:O	2.16	0.46
1:A:172:LYS:HG2	1:A:176:LYS:NZ	2.29	0.46
1:A:82:GLN:NE2	1:A:126:HIS:HB2	2.31	0.46
1:A:185:ASN:HA	1:A:294:ASN:O	2.16	0.45
1:A:349:ASN:C	1:A:349:ASN:HD22	2.24	0.45
1:A:222:ASP:OD1	1:A:222:ASP:C	2.60	0.45
1:A:108:MET:HG2	1:A:114:PHE:CE2	2.52	0.44
1:A:311:LYS:HD3	1:A:313:HIS:CE1	2.53	0.44
1:A:121:GLU:HG2	1:A:123:MET:HE2	1.99	0.44
1:A:232:VAL:HG11	1:A:324:LYS:HG3	2.00	0.43
1:A:108:MET:HE3	1:A:114:PHE:CE2	2.53	0.43
1:A:223:GLN:HE21	1:A:258:VAL:CG2	2.32	0.43
1:A:109:ALA:O	1:A:110:ASN:C	2.62	0.42
1:A:227:LEU:HD13	1:A:278:TRP:CG	2.54	0.42
1:A:103:TYR:CD2	1:A:114:PHE:CZ	3.09	0.41
1:A:223:GLN:HE22	1:A:258:VAL:HG22	1.85	0.41
1:A:103:TYR:CD2	1:A:114:PHE:HZ	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:MET:HE3	1:A:114:PHE:CD2	2.55	0.41

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	335/349 (96%)	311 (93%)	20 (6%)	4 (1%)	10 12

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	ASN
1	A	304	LYS
1	A	310	LEU
1	A	309	PRO

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	297/304 (98%)	269 (91%)	28 (9%)	8 11

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	29	GLU
1	A	40	ARG
1	A	47	GLN
1	A	53	GLU
1	A	75	LYS
1	A	85	ILE
1	A	87	ASN
1	A	99	LYS
1	A	106	LYS
1	A	133	GLN
1	A	138	ARG
1	A	149	THR
1	A	154	VAL
1	A	156	ARG
1	A	159	VAL
1	A	172	LYS
1	A	181	GLN
1	A	258	VAL
1	A	275	MET
1	A	285	LEU
1	A	289	ILE
1	A	305	ARG
1	A	306	ILE
1	A	307	GLU
1	A	310	LEU
1	A	334	GLN
1	A	349	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	82	GLN
1	A	126	HIS
1	A	133	GLN
1	A	137	GLN
1	A	194	ASN
1	A	205	ASN
1	A	223	GLN
1	A	254	ASN
1	A	257	ASN
1	A	313	HIS

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Mol	Chain	Res	Type
1	A	321	ASN
1	A	334	GLN
1	A	349	ASN

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](#)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 for Mogul analysis.

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	FUM	A	351	2	7,7,7	1.32	2 (28%)	8,8,8	1.01	0
4	SO4	A	1353	-	4,4,4	0.20	0	6,6,6	0.37	0
4	SO4	A	1352	-	4,4,4	0.27	0	6,6,6	0.27	0
4	SO4	A	1354[A]	-	4,4,4	0.18	0	6,6,6	1.17	0
4	SO4	A	1354[B]	-	4,4,4	0.15	0	6,6,6	0.81	0
4	SO4	A	1355	-	4,4,4	0.34	0	6,6,6	0.35	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
3	FUM	A	351	2	-	0/5/5/5	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	351	FUM	O7-C6	2.27	1.28	1.23
3	A	351	FUM	O-C	2.02	1.28	1.23

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	339/349 (97%)	1.17	74 (21%) 2 2	31, 46, 90, 99	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	87	ASN	5.7
1	A	12	GLY	5.5
1	A	110	ASN	5.0
1	A	11	SER	4.7
1	A	139	GLY	4.6
1	A	115	LYS	4.6
1	A	9	VAL	4.3
1	A	306	ILE	4.3
1	A	140	GLY	4.3
1	A	96	SER	4.2
1	A	111	PHE	4.0
1	A	114	PHE	3.9
1	A	292	THR	3.7
1	A	109	ALA	3.6
1	A	90	PHE	3.6
1	A	305	ARG	3.6
1	A	132	LEU	3.6
1	A	86	GLY	3.4
1	A	119	ASN	3.4
1	A	8	ALA	3.3
1	A	106	LYS	3.3
1	A	162	PHE	3.3
1	A	85	ILE	3.1
1	A	103	TYR	3.0
1	A	308	TYR	3.0
1	A	129	VAL	3.0
1	A	291	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	13	SER	3.0
1	A	101	LEU	2.9
1	A	260	GLY	2.9
1	A	153	THR	2.9
1	A	155	GLY	2.8
1	A	135	ILE	2.8
1	A	104	ASP	2.8
1	A	10	ALA	2.8
1	A	123	MET	2.8
1	A	293	VAL	2.8
1	A	14	GLY	2.8
1	A	125	PHE	2.8
1	A	108	MET	2.7
1	A	154	VAL	2.7
1	A	304	LYS	2.7
1	A	286	ASN	2.7
1	A	131	LYS	2.7
1	A	94	SER	2.7
1	A	250	GLU	2.5
1	A	152	ASP	2.5
1	A	296	TRP	2.5
1	A	294	ASN	2.5
1	A	26	ALA	2.5
1	A	82	GLN	2.5
1	A	29	GLU	2.4
1	A	141	GLU	2.4
1	A	300	ALA	2.4
1	A	149	THR	2.3
1	A	151	ASN	2.3
1	A	142	GLU	2.3
1	A	144	LEU	2.3
1	A	88	GLY	2.3
1	A	138	ARG	2.3
1	A	102	TYR	2.2
1	A	83	GLU	2.2
1	A	22	ALA	2.2
1	A	301	PRO	2.2
1	A	181	GLN	2.2
1	A	309	PRO	2.2
1	A	19	GLU	2.2
1	A	71	TYR	2.1
1	A	113	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	92	VAL	2.1
1	A	133	GLN	2.1
1	A	328	GLU	2.1
1	A	27	TRP	2.1
1	A	130	GLU	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(Å ²)	Q<0.9
4	SO4	A	1352	5/5	0.58	0.16	149,150,150,150	0
4	SO4	A	1353	5/5	0.72	0.16	141,141,142,142	0
4	SO4	A	1355	5/5	0.83	0.11	97,98,99,100	0
4	SO4	A	1354[B]	5/5	0.89	0.23	59,61,64,69	5
4	SO4	A	1354[A]	5/5	0.89	0.23	60,62,65,67	5
3	FUM	A	351	8/8	0.94	0.09	39,43,45,50	0
2	FE	A	350	1/1	0.99	0.08	46,46,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.