



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 01:14 PM GMT

PDB ID : 3ONW
Title : Structure of a G-alpha-i1 mutant with enhanced affinity for the RGS14 GoLoco motif.
Authors : Bosch, D.; Kimple, A.J.; Sammond, D.W.; Miley, M.J.; Machius, M.; Kuhlman, B.; Willard, F.S.; Siderovski, D.P.
Deposited on : 2010-08-30
Resolution : 2.38 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

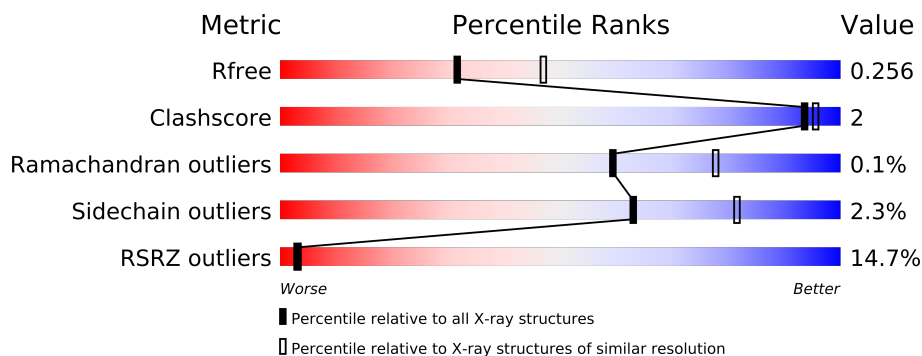
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.38 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}	66092	2963 (2.40-2.36)
Clashscore	79885	3668 (2.40-2.36)
Ramachandran outliers	78287	3600 (2.40-2.36)
Sidechain outliers	78261	3602 (2.40-2.36)
RSRZ outliers	66119	2966 (2.40-2.36)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	328	
1	B	328	
2	C	36	
2	D	36	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	SO4	A	3	-	X
4	SO4	B	1	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5811 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Guanine nucleotide-binding protein G(i) subunit alpha-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	0	0
			2543	1617	428	483	15			
1	B	317	Total	C	N	O	S	0	0	0
			2551	1623	429	484	15			

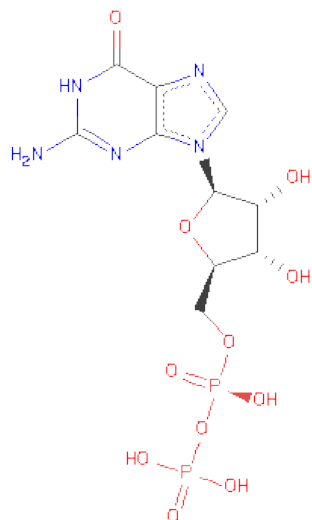
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	SER	-	EXPRESSION TAG	UNP P63096
A	28	ASN	-	EXPRESSION TAG	UNP P63096
A	29	ALA	-	EXPRESSION TAG	UNP P63096
A	30	GLY	-	EXPRESSION TAG	UNP P63096
A	147	LEU	GLN	ENGINEERED MUTATION	UNP P63096
B	27	SER	-	EXPRESSION TAG	UNP P63096
B	28	ASN	-	EXPRESSION TAG	UNP P63096
B	29	ALA	-	EXPRESSION TAG	UNP P63096
B	30	GLY	-	EXPRESSION TAG	UNP P63096
B	147	LEU	GLN	ENGINEERED MUTATION	UNP P63096

- Molecule 2 is a protein called Regulator of G-protein signaling 14.

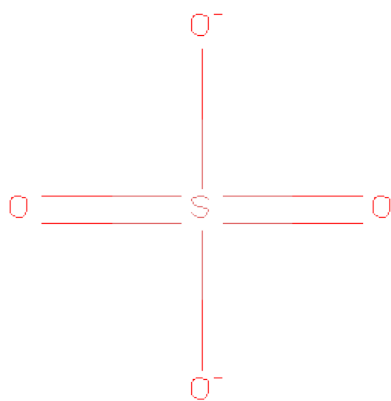
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	35	Total	C	N	O	0	0	0
			279	175	51	53			
2	D	34	Total	C	N	O	0	0	0
			270	168	49	53			

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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

- Molecule 5 is water.

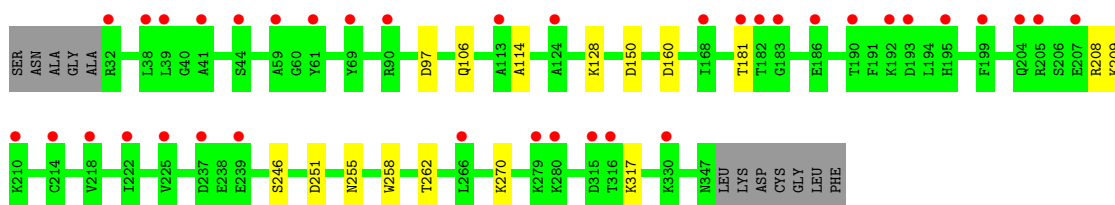
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	52	Total	O	0	0
			52	52		
5	B	40	Total	O	0	0
			40	40		
5	C	2	Total	O	0	0
			2	2		
5	D	3	Total	O	0	0
			3	3		

3 Residue-property plots

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.

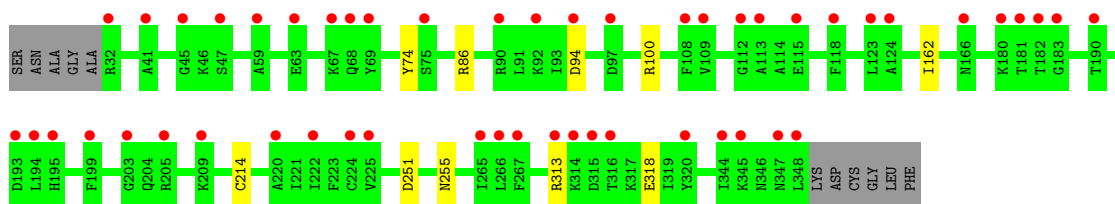
- Molecule 1: Guanine nucleotide-binding protein G(i) subunit alpha-1

Chain A: 



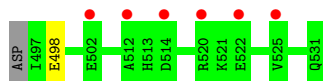
- Molecule 1: Guanine nucleotide-binding protein G(i) subunit alpha-1

Chain B: 



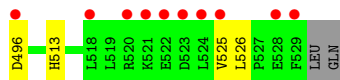
- Molecule 2: Regulator of G-protein signaling 14

Chain C: 



- Molecule 2: Regulator of G-protein signaling 14

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	70.39Å 83.68Å 190.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	95.07 – 2.38 28.88 – 2.38	Depositor EDS
% Data completeness (in resolution range)	98.5 (95.07-2.38) 98.6 (28.88-2.38)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.228 , 0.265 0.222 , 0.256	Depositor DCC
R_{free} test set	1528 reflections (3.49%)	DCC
Wilson B-factor (Å ²)	53.7	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 45283 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5811	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, 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	0.48	0/2589	0.55	0/3488
1	B	0.46	0/2597	0.53	0/3499
2	C	0.43	0/281	0.52	0/377
2	D	0.42	0/272	0.56	0/365
All	All	0.47	0/5739	0.54	0/7729

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2543	0	0	5	0
1	B	2551	0	0	4	0
2	C	279	0	0	0	0
2	D	270	0	0	1	0
3	A	28	0	0	0	0
3	B	28	0	0	0	0
4	A	5	0	0	0	0
4	B	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	52	0	0	1	0
5	B	40	0	0	0	0
5	C	2	0	0	0	0
5	D	3	0	0	0	0
All	All	5811	0	0	9	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (9) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:251:ASP:OD1	1:A:255:ASN:ND2	2.40	0.55
1:B:251:ASP:OD1	1:B:255:ASN:ND2	2.41	0.53
1:B:74:TYR:OH	1:B:162:ILE:O	2.27	0.53
1:A:262:THR:O	1:A:317:LYS:NZ	2.51	0.44
1:A:128:LYS:NZ	1:A:160:ASP:OD1	2.51	0.43
1:B:255:ASN:O	1:B:313:ARG:NH2	2.51	0.43
1:A:150:ASP:OD2	1:A:270:LYS:NZ	2.51	0.43
1:B:86:ARG:NH2	2:D:525:VAL:O	2.52	0.43
1:A:208:ARG:NE	5:A:394:HOH:O	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	314/328 (96%)	308 (98%)	5 (2%)	1 (0%)	50	66
1	B	315/328 (96%)	306 (97%)	9 (3%)	0	100	100
2	C	33/36 (92%)	32 (97%)	1 (3%)	0	100	100
2	D	32/36 (89%)	30 (94%)	2 (6%)	0	100	100
All	All	694/728 (95%)	676 (97%)	17 (2%)	1 (0%)	59	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	ALA

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	275/283 (97%)	269 (98%)	6 (2%)	64	83
1	B	276/283 (98%)	272 (99%)	4 (1%)	78	91
2	C	31/32 (97%)	30 (97%)	1 (3%)	51	71
2	D	30/32 (94%)	27 (90%)	3 (10%)	11	15
All	All	612/630 (97%)	598 (98%)	14 (2%)	63	81

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	ASP
1	A	106	GLN
1	A	181	THR
1	A	209	LYS
1	A	246	SER
1	A	258	TRP
1	B	94	ASP
1	B	100	ARG
1	B	214	CYS
1	B	318	GLU
2	C	498	GLU
2	D	496	ASP
2	D	513	HIS
2	D	526	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

5 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	$\# Z > 2$
4	SO4	A	3	-	4,4,4	0.18	0	6,6,6	0.05	0
3	GDP	A	401	-	30,30,30	1.41	3 (10%)	44,47,47	3.11	9 (20%)
4	SO4	B	1	-	4,4,4	0.18	0	6,6,6	0.18	0
4	SO4	B	2	-	4,4,4	0.13	0	6,6,6	0.06	0
3	GDP	B	401	-	30,30,30	1.32	4 (13%)	44,47,47	3.11	9 (20%)

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
4	SO4	A	3	-	-	0/0/0/0	0/0/0/0
3	GDP	A	401	-	-	0/16/32/32	0/1/3/3
4	SO4	B	1	-	-	0/0/0/0	0/0/0/0
4	SO4	B	2	-	-	0/0/0/0	0/0/0/0
3	GDP	B	401	-	-	0/16/32/32	0/1/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	GDP	C6-C5	4.28	1.48	1.41
3	B	401	GDP	C4-N9	-3.51	1.32	1.37
3	B	401	GDP	C6-C5	3.29	1.46	1.41
3	A	401	GDP	C5-C4	2.87	1.47	1.40
3	B	401	GDP	C5-C4	2.82	1.46	1.40
3	A	401	GDP	C4-N9	-2.54	1.34	1.37
3	B	401	GDP	C2-N2	2.00	1.35	1.32

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	GDP	C6-C5-N7	17.25	136.46	134.14
3	B	401	GDP	C6-C5-N7	16.95	136.42	134.14
3	B	401	GDP	O4'-C1'-N9	-5.17	103.63	108.44
3	A	401	GDP	N3-C4-N9	5.14	134.45	126.91
3	B	401	GDP	N3-C4-N9	4.65	133.73	126.91
3	A	401	GDP	C5-C4-N3	-4.30	119.71	125.94
3	B	401	GDP	C8-N9-C4	3.98	109.94	106.90
3	A	401	GDP	C2-N3-C4	3.90	120.56	115.09
3	B	401	GDP	C5-C4-N3	-3.67	120.62	125.94
3	A	401	GDP	PA-O3A-PB	-3.65	120.99	131.68
3	B	401	GDP	C2-N3-C4	3.29	119.71	115.09
3	A	401	GDP	C8-N9-C4	3.25	109.38	106.90
3	B	401	GDP	C1'-N9-C4	-2.84	121.72	126.64
3	B	401	GDP	C4-C5-N7	-2.83	107.10	109.52
3	A	401	GDP	C4-C5-N7	-2.80	107.13	109.52
3	B	401	GDP	PA-O3A-PB	-2.77	123.57	131.68
3	A	401	GDP	O4'-C1'-N9	-2.64	105.98	108.44
3	A	401	GDP	C1'-N9-C4	-2.48	122.36	126.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	316/328 (96%)	0.65	37 (11%) 5 6	33, 59, 85, 97	0
1	B	317/328 (96%)	0.83	51 (16%) 2 2	31, 60, 90, 102	0
2	C	35/36 (97%)	1.17	6 (17%) 2 2	60, 78, 91, 101	0
2	D	34/36 (94%)	1.25	10 (29%) 1 1	51, 80, 102, 108	0
All	All	702/728 (96%)	0.79	104 (14%) 3 3	31, 61, 90, 108	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	348	LEU	9.3
1	B	182	THR	8.0
1	A	182	THR	6.4
1	A	193	ASP	5.4
1	B	315	ASP	5.3
1	B	113	ALA	5.3
1	A	315	ASP	5.1
1	B	118	PHE	4.6
2	C	512	ALA	4.5
1	B	183	GLY	4.4
2	D	525	VAL	4.3
1	B	59	ALA	4.2
1	B	181	THR	4.2
1	A	168	ILE	4.2
1	B	203	GLY	4.1
1	B	190	THR	4.0
1	A	222	ILE	3.9
1	B	344	ILE	3.9
2	D	496	ASP	3.9
1	B	112	GLY	3.5
1	A	205	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	69	TYR	3.4
1	B	109	VAL	3.3
1	B	347	ASN	3.3
1	B	63	GLU	3.3
1	A	113	ALA	3.2
1	B	195	HIS	3.2
1	A	186	GLU	3.2
2	D	522	GLU	3.1
1	A	90	ARG	3.1
1	A	61	TYR	3.1
1	B	180	LYS	3.0
1	A	32	ARG	3.0
2	D	523	ASP	2.9
2	D	524	LEU	2.8
1	A	207	GLU	2.8
2	C	522	GLU	2.8
1	B	32	ARG	2.8
1	B	193	ASP	2.7
2	C	514	ASP	2.7
1	B	314	LYS	2.7
2	C	525	VAL	2.6
1	B	92	LYS	2.6
1	B	94	ASP	2.6
1	B	267	PHE	2.6
1	B	224	CYS	2.6
1	A	330	LYS	2.6
1	A	192	LYS	2.6
1	A	69	TYR	2.6
1	A	199	PHE	2.6
2	D	529	PHE	2.5
1	B	115	GLU	2.5
1	B	320	TYR	2.5
1	A	195	HIS	2.5
1	B	209	LYS	2.5
1	B	345	LYS	2.5
2	C	520	ARG	2.5
1	A	190	THR	2.4
1	B	75	SER	2.4
1	B	166	ASN	2.4
1	B	67	LYS	2.4
1	A	218	VAL	2.4
1	A	44	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	199	PHE	2.4
1	A	239	GLU	2.4
1	A	124	ALA	2.3
2	D	521	LYS	2.3
1	A	183	GLY	2.3
1	A	59	ALA	2.3
1	B	68	GLN	2.3
1	B	124	ALA	2.3
1	B	313	ARG	2.2
1	A	38	LEU	2.2
1	A	266	LEU	2.2
1	B	316	THR	2.2
1	A	225	VAL	2.2
2	C	502	GLU	2.2
1	A	181	THR	2.2
1	A	279	LYS	2.2
2	D	528	GLU	2.2
1	A	316	THR	2.2
1	B	41	ALA	2.2
1	B	266	LEU	2.2
1	B	205	ARG	2.1
1	B	108	PHE	2.1
1	A	39	LEU	2.1
1	B	47	SER	2.1
1	B	225	VAL	2.1
1	B	90	ARG	2.1
1	B	45	GLY	2.1
1	A	204	GLN	2.1
1	B	194	LEU	2.1
1	B	222	ILE	2.1
2	D	520	ARG	2.1
1	A	280	LYS	2.1
1	A	210	LYS	2.1
1	B	97	ASP	2.1
1	B	265	ILE	2.1
1	A	214	CYS	2.0
1	B	220	ALA	2.0
1	B	123	LEU	2.0
1	A	237	ASP	2.0
1	A	41	ALA	2.0
2	D	518	LEU	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 carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	SO4	A	3	5/5	0.33	4.13	120,120,121,121	0
4	SO4	B	1	5/5	0.25	2.44	84,85,85,86	0
4	SO4	B	2	5/5	0.23	1.91	99,100,100,100	0
3	GDP	B	401	28/28	0.22	0.87	41,46,49,49	0
3	GDP	A	401	28/28	0.16	-0.26	40,44,48,49	0

6.5 Other polymers ⓘ

There are no such residues in this entry.