



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:47 PM GMT

PDB ID : 4G5Q
Title : Structure of LGN GL4/Galphai1 complex
Authors : Jia, M.; Li, J.; Zhu, J.; Wen, W.; Zhang, M.; Wang, W.
Deposited on : 2012-07-18
Resolution : 2.90 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

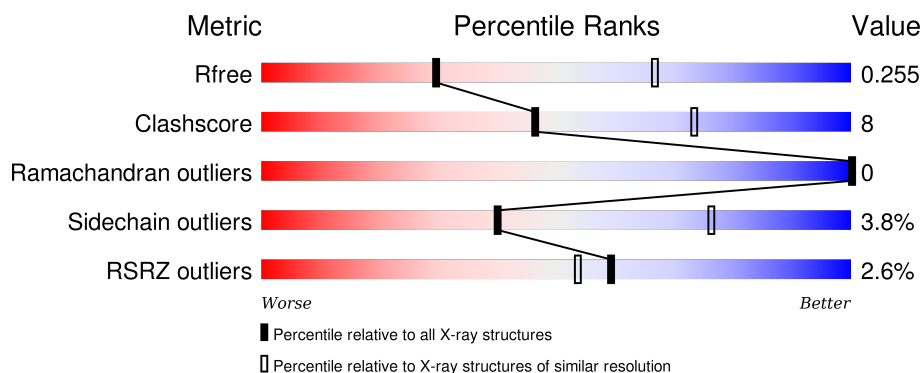
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION




The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	330	 84% 12% ..
1	B	330	 85% 9% ..
1	C	330	 78% 16% ..
1	D	330	 84% 12% ..
2	E	25	 60% 16% 8% 16%

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Mol	Chain	Length	Quality of chain
2	F	25	 64% 20% 12%
2	G	25	 64% 28% 12%
2	H	25	 64% 24% 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	B	406	-	-	-	X
5	CIT	C	402	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11211 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 Guanine nucleotide-binding protein G(i) subunit alpha-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	1	0
			2545	1616	425	488	16			
1	B	316	Total	C	N	O	S	0	1	0
			2524	1607	419	482	16			
1	C	316	Total	C	N	O	S	0	0	0
			2539	1620	423	480	16			
1	D	324	Total	C	N	O	S	0	1	0
			2579	1642	431	490	16			

- Molecule 2 is a protein called G-protein-signaling modulator 2.

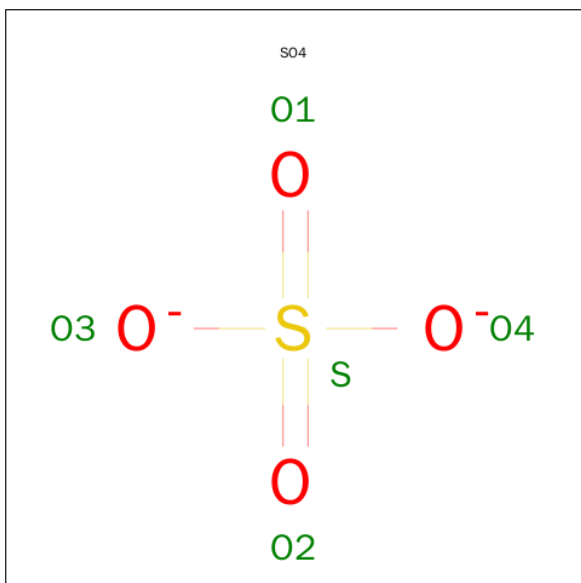
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	21	Total	C	N	O	S	0	0	0
			175	111	32	31	1			
2	F	22	Total	C	N	O	S	0	0	0
			184	117	34	32	1			
2	G	24	Total	C	N	O	S	0	0	0
			200	125	38	36	1			
2	H	22	Total	C	N	O	S	0	0	0
			181	116	34	30	1			

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



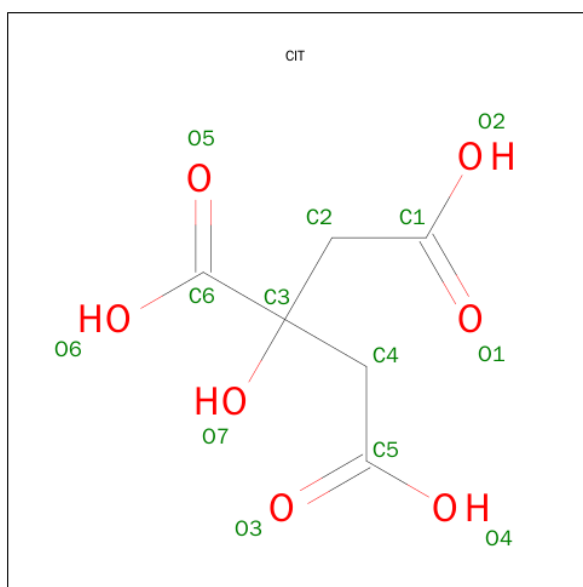
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 28	C 10	N 5	O 11	P 2	0	0
3	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
3	C	1	Total 28	C 10	N 5	O 11	P 2	0	0
3	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

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



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

- Molecule 5 is CITRIC ACID (three-letter code: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			13	6	7		
5	B	1	Total	C	O	0	0
			13	6	7		
5	C	1	Total	C	O	0	0
			13	6	7		
5	D	1	Total	C	O	0	0
			13	6	7		

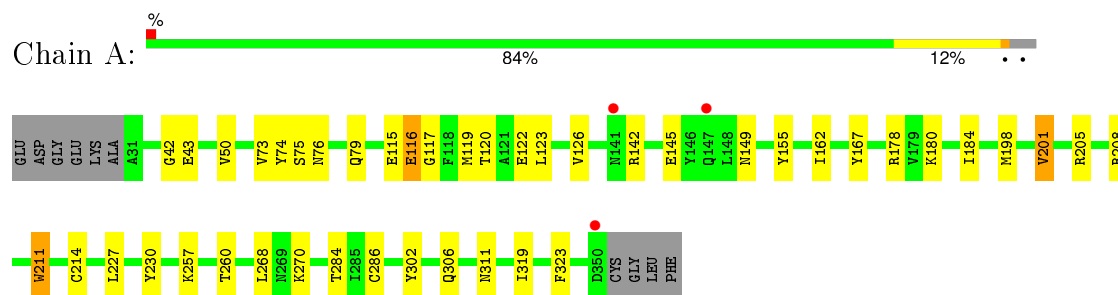
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	7	Total	O	0	0
			7	7		
6	B	8	Total	O	0	0
			8	8		
6	C	9	Total	O	0	0
			9	9		
6	D	7	Total	O	0	0
			7	7		
6	E	1	Total	O	0	0
			1	1		
6	F	1	Total	O	0	0
			1	1		
6	G	2	Total	O	0	0
			2	2		

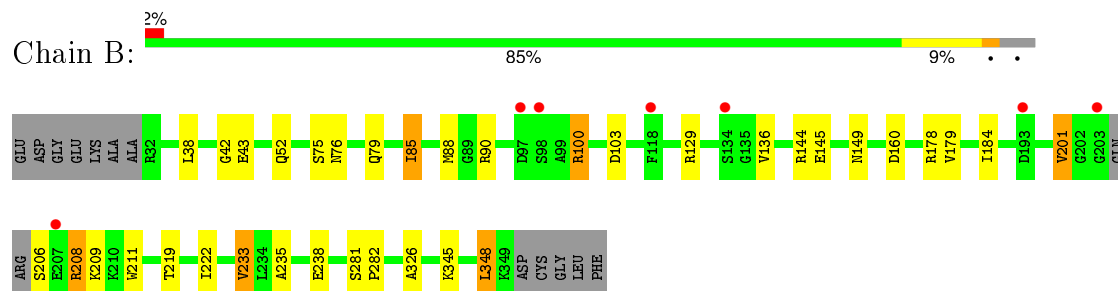
3 Residue-property plots [i](#)

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.

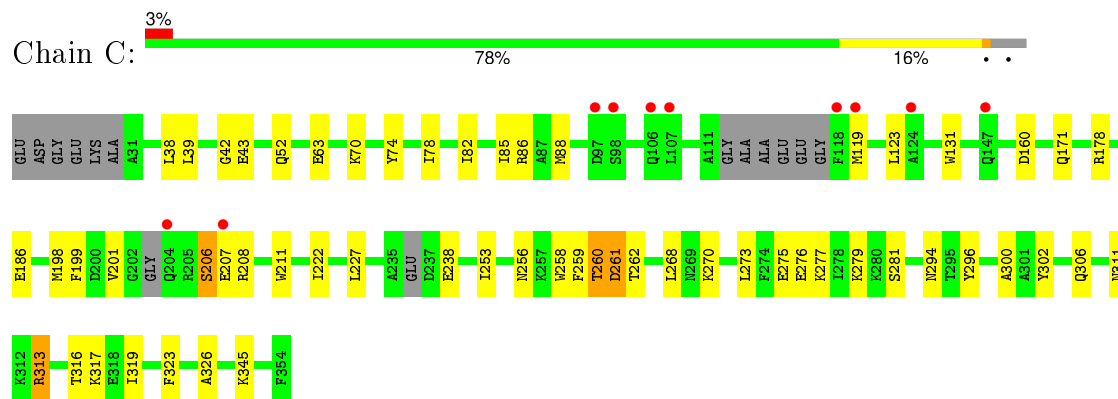
- Molecule 1: Guanine nucleotide-binding protein G(i) subunit alpha-1



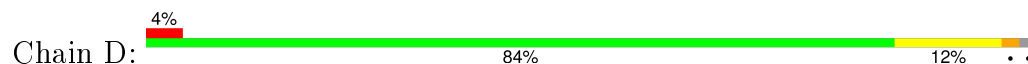
- Molecule 1: Guanine nucleotide-binding protein G(i) subunit alpha-1

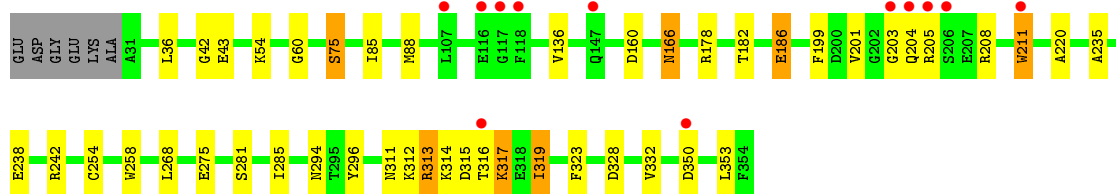


- Molecule 1: Guanine nucleotide-binding protein G(i) subunit alpha-1



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





• Molecule 2: G-protein-signaling modulator 2

Chain E: 60% 16% 8% 16%



• Molecule 2: G-protein-signaling modulator 2

Chain F: 64% 20% 12%



• Molecule 2: G-protein-signaling modulator 2

Chain G: 8% 64% 28% 2%



• Molecule 2: G-protein-signaling modulator 2

Chain H: 4% 64% 24% 12%



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	207.38 Å 207.38 Å 236.66 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.90 49.81 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-2.90) 99.9 (49.81-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.47 (at 2.91 Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.207 , 0.243 0.219 , 0.255	Depositor DCC
R_{free} test set	3384 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	60.3	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 66861 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11211	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, SO4, CIT

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	0.53	1/2593 (0.0%)	0.64	0/3499
1	B	0.55	0/2572	0.63	0/3468
1	C	0.54	2/2583 (0.1%)	0.62	0/3478
1	D	0.54	2/2630 (0.1%)	0.62	1/3549 (0.0%)
2	E	0.53	0/176	0.88	0/234
2	F	0.61	0/185	0.85	0/245
2	G	0.52	0/201	0.72	0/267
2	H	0.42	0/182	0.66	0/241
All	All	0.54	5/11122 (0.0%)	0.64	1/14981 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	211	TRP	CD2-CE2	5.70	1.48	1.41
1	A	211	TRP	CD2-CE2	5.47	1.48	1.41
1	C	131	TRP	CD2-CE2	5.32	1.47	1.41
1	C	211	TRP	CD2-CE2	5.26	1.47	1.41
1	D	258	TRP	CD2-CE2	5.11	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	D	350	ASP	CB-CG-OD2	5.22	123.00	118.30

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	2545	0	2495	40	0
1	B	2524	0	2480	37	0
1	C	2539	0	2509	35	0
1	D	2579	0	2526	39	0
2	E	175	0	176	7	0
2	F	184	0	189	8	0
2	G	200	0	197	5	0
2	H	181	0	187	4	0
3	A	28	0	12	1	0
3	B	28	0	12	0	0
3	C	28	0	12	1	0
3	D	28	0	12	0	0
4	A	20	0	0	0	0
4	B	20	0	0	0	0
4	C	20	0	0	1	0
4	D	25	0	0	1	0
5	B	26	0	10	1	0
5	C	13	0	5	3	0
5	D	13	0	5	0	0
6	A	7	0	0	0	0
6	B	8	0	0	0	0
6	C	9	0	0	0	0
6	D	7	0	0	1	0
6	E	1	0	0	3	0
6	F	1	0	0	4	0
6	G	2	0	0	3	0
All	All	11211	0	10827	167	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 8.

All (167) 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:B:208:ARG:NH1	1:B:208:ARG:HB2	1.68	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:ARG:HB2	1:B:208:ARG:HH11	1.17	1.05
2:E:635:ARG:HB3	6:E:701:HOH:O	1.60	0.99
1:C:260:THR:HG22	1:C:261:ASP:OD1	1.60	0.99
1:C:313:ARG:HH22	1:C:317:LYS:HE2	1.35	0.90
1:B:208:ARG:CB	1:B:208:ARG:NH1	2.35	0.88
5:C:402:CIT:H41	5:C:402:CIT:O2	1.74	0.87
2:G:640:ARG:HD2	6:G:701:HOH:O	1.75	0.85
2:F:640:ARG:HD2	6:F:701:HOH:O	1.77	0.83
1:B:345:LYS:O	1:B:348:LEU:HD12	1.83	0.79
1:A:205:ARG:HB2	2:E:629:LEU:HD11	1.68	0.74
1:A:142:ARG:HD2	1:A:145:GLU:OE2	1.86	0.74
1:D:201:VAL:HG13	1:D:211:TRP:NE1	2.03	0.74
1:B:184:ILE:HD11	1:B:211:TRP:HA	1.71	0.73
1:D:294:ASN:HB2	6:D:507:HOH:O	1.89	0.71
1:A:43:GLU:OE1	1:A:178:ARG:NH1	2.25	0.70
1:A:116:GLU:CD	1:A:116:GLU:H	1.94	0.70
5:C:402:CIT:C4	5:C:402:CIT:O2	2.39	0.70
1:D:315:ASP:O	1:D:316:THR:OG1	2.08	0.70
1:D:85:ILE:HA	1:D:88:MET:HE3	1.74	0.69
2:G:635:ARG:HB3	6:G:701:HOH:O	1.92	0.69
1:D:42:GLY:O	1:D:43:GLU:HB2	1.91	0.69
1:A:74:TYR:CD1	1:A:119:MET:HE3	2.27	0.69
1:D:281:SER:HB3	1:D:285:ILE:HD12	1.73	0.69
1:B:76:ASN:HA	1:B:79:GLN:HE21	1.57	0.68
1:B:208:ARG:CB	1:B:208:ARG:CZ	2.71	0.68
2:F:636:MET:N	6:F:701:HOH:O	2.08	0.66
1:D:75:SER:HB3	2:H:641:VAL:HG21	1.77	0.66
1:A:116:GLU:N	1:A:116:GLU:CD	2.49	0.66
2:E:640:ARG:HD2	6:E:701:HOH:O	1.96	0.65
1:A:76:ASN:HA	1:A:79:GLN:HE21	1.61	0.64
1:B:100:ARG:NH1	1:B:103:ASP:OD2	2.30	0.64
2:F:635:ARG:HB3	2:F:640:ARG:HH11	1.64	0.63
1:B:208:ARG:HB3	1:B:208:ARG:CZ	2.29	0.63
2:F:635:ARG:CB	6:F:701:HOH:O	2.47	0.62
1:B:144:ARG:O	1:B:233:VAL:HG12	1.99	0.62
2:G:635:ARG:CB	6:G:701:HOH:O	2.47	0.61
1:B:75:SER:HB3	2:F:641:VAL:HG21	1.82	0.60
1:C:38:LEU:HD23	1:C:222:ILE:HB	1.83	0.60
2:F:635:ARG:HB3	6:F:701:HOH:O	2.02	0.60
1:C:43:GLU:OE1	1:C:178:ARG:NH1	2.35	0.60
1:B:345:LYS:HA	1:B:348:LEU:HD11	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:ARG:HG3	1:B:209:LYS:N	2.17	0.59
1:A:116:GLU:OE2	1:A:117:GLY:N	2.36	0.59
1:D:186:GLU:HG3	1:D:199:PHE:CE1	2.39	0.58
1:B:85:ILE:HA	1:B:88:MET:HE3	1.86	0.58
1:B:38:LEU:HD23	1:B:222:ILE:HB	1.85	0.58
1:C:238:GLU:HA	1:C:238:GLU:OE1	2.03	0.57
1:A:149:ASN:OD1	1:A:178:ARG:HD2	2.03	0.57
1:C:52:GLN:NE2	1:C:326:ALA:O	2.37	0.57
1:A:43:GLU:CD	1:A:178:ARG:HH12	2.07	0.57
1:C:206:SER:O	1:C:207:GLU:HB2	2.05	0.56
1:C:85:ILE:HG13	1:C:88:MET:CE	2.36	0.56
1:C:294:ASN:HB2	4:C:406:SO4:O4	2.06	0.56
1:C:119:MET:HG3	1:C:123:LEU:HD23	1.88	0.55
1:A:50:VAL:HG22	1:A:198:MET:HE3	1.88	0.55
1:B:145:GLU:HA	1:B:233:VAL:CG1	2.36	0.55
1:D:201:VAL:CG1	1:D:211:TRP:NE1	2.70	0.55
1:A:180:LYS:HE3	2:E:637:ASP:HB3	1.89	0.55
1:D:313:ARG:O	1:D:317:LYS:HB3	2.07	0.55
1:A:74:TYR:CE1	1:A:119:MET:HE3	2.42	0.55
1:C:313:ARG:NH2	1:C:317:LYS:HE2	2.16	0.54
2:H:628:ILE:O	2:H:632:GLN:HG3	2.07	0.54
1:B:76:ASN:HD22	1:B:79:GLN:HE22	1.55	0.53
1:B:76:ASN:HD22	1:B:79:GLN:NE2	2.06	0.53
1:A:260:THR:HG21	1:C:208:ARG:HH11	1.74	0.53
1:C:260:THR:CG2	1:C:261:ASP:OD1	2.48	0.53
1:D:275:GLU:HG3	1:D:296:TYR:CG	2.44	0.53
1:C:186:GLU:HG3	1:C:199:PHE:CE1	2.44	0.52
1:A:184:ILE:HD11	1:A:211:TRP:HA	1.91	0.52
1:D:268:LEU:HD12	1:D:323:PHE:CE2	2.43	0.52
1:C:275:GLU:HG3	1:C:296:TYR:CG	2.45	0.52
1:B:345:LYS:HA	1:B:348:LEU:CD1	2.40	0.52
1:B:43:GLU:CD	1:B:178:ARG:HH12	2.13	0.51
1:D:311:ASN:HB2	1:D:319:ILE:CD1	2.40	0.51
1:A:205:ARG:HD3	1:A:208:ARG:HE	1.74	0.51
1:C:39:LEU:HD13	1:C:253:ILE:HD13	1.91	0.51
1:A:123:LEU:HD12	1:A:123:LEU:O	2.11	0.51
1:B:235:ALA:HB3	1:B:238:GLU:HG3	1.92	0.51
1:D:166:ASN:H	1:D:166:ASN:ND2	2.08	0.51
1:D:88:MET:HE1	1:D:136:VAL:HG22	1.92	0.51
1:C:70:LYS:HE2	1:C:74:TYR:HE2	1.74	0.50
1:B:42:GLY:O	1:B:43:GLU:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:THR:CG2	1:C:208:ARG:HH11	2.25	0.50
1:A:178:ARG:NH2	2:E:640:ARG:HG2	2.27	0.49
1:C:276:GLU:OE2	1:C:279:LYS:NZ	2.46	0.49
1:C:42:GLY:O	1:C:43:GLU:HB2	2.12	0.49
1:C:300:ALA:HB1	1:C:323:PHE:CE2	2.48	0.49
1:D:186:GLU:HG3	1:D:199:PHE:CD1	2.47	0.49
1:A:116:GLU:N	1:A:116:GLU:OE2	2.44	0.48
1:A:122:GLU:O	1:A:126:VAL:HG23	2.12	0.48
1:C:311:ASN:HB2	1:C:319:ILE:HD11	1.95	0.48
1:A:116:GLU:CA	1:A:116:GLU:OE2	2.62	0.48
1:B:43:GLU:OE1	1:B:178:ARG:NH1	2.47	0.48
1:A:119:MET:O	1:A:120:THR:C	2.51	0.48
1:D:328:ASP:O	1:D:332:VAL:HG23	2.14	0.48
1:A:323:PHE:O	5:B:402:CIT:O5	2.32	0.47
1:A:162:ILE:HG22	1:A:167:TYR:CZ	2.49	0.47
1:C:273:LEU:O	1:C:277:LYS:HG3	2.15	0.47
1:A:76:ASN:HD22	1:A:79:GLN:NE2	2.12	0.47
1:A:115:GLU:O	1:A:115:GLU:HG2	2.15	0.47
1:D:314:LYS:HA	1:D:315:ASP:HA	1.69	0.47
1:B:209:LYS:HE2	1:B:209:LYS:HB3	1.33	0.47
1:D:201:VAL:CG1	1:D:211:TRP:CE2	2.97	0.47
1:D:315:ASP:HA	1:D:317:LYS:HZ3	1.80	0.47
1:B:76:ASN:HA	1:B:79:GLN:NE2	2.27	0.47
1:A:42:GLY:O	1:A:43:GLU:HB2	2.15	0.46
1:D:182:THR:HA	1:D:204:GLN:OE1	2.15	0.46
2:F:635:ARG:HB3	2:F:640:ARG:NH1	2.27	0.46
1:A:74:TYR:CD1	1:A:119:MET:CE	2.98	0.46
1:D:182:THR:O	1:D:204:GLN:HB2	2.15	0.46
1:D:314:LYS:CB	1:D:317:LYS:NZ	2.79	0.46
1:D:281:SER:HB3	1:D:285:ILE:CD1	2.41	0.46
1:C:302:TYR:O	1:C:306:GLN:HG2	2.16	0.46
1:A:142:ARG:CD	1:A:145:GLU:OE2	2.62	0.46
1:A:227:LEU:HD21	1:A:268:LEU:HB3	1.98	0.46
1:D:205:ARG:HD3	1:D:208:ARG:CB	2.46	0.46
1:D:314:LYS:CB	1:D:317:LYS:HZ2	2.28	0.46
1:C:38:LEU:HD11	1:C:198:MET:HE3	1.97	0.46
1:C:70:LYS:HE2	1:C:74:TYR:CE2	2.50	0.46
1:B:52:GLN:NE2	1:B:326:ALA:O	2.43	0.45
1:D:42:GLY:O	1:D:43:GLU:CB	2.63	0.45
1:B:88:MET:CE	1:B:136:VAL:HG22	2.46	0.45
1:D:203:GLY:HA3	2:H:633:ALA:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:TYR:N	5:C:402:CIT:O1	2.49	0.45
1:B:201:VAL:HG13	1:B:211:TRP:HE1	1.81	0.45
2:G:622:GLU:OE1	2:G:630:ARG:NH1	2.48	0.45
1:D:201:VAL:O	1:D:201:VAL:CG1	2.61	0.45
1:B:75:SER:CB	2:F:641:VAL:HG21	2.46	0.45
1:A:311:ASN:HB2	1:A:319:ILE:HD11	1.98	0.45
1:C:39:LEU:CD1	1:C:253:ILE:HD13	2.46	0.45
1:A:73:VAL:HG13	1:A:155:TYR:CE1	2.52	0.44
1:C:259:PHE:HB3	1:C:262:THR:HB	1.99	0.44
1:D:43:GLU:OE2	1:D:178:ARG:NH1	2.48	0.44
1:D:88:MET:HE2	1:D:88:MET:HB2	1.84	0.44
1:C:256:ASN:OD1	1:C:258:TRP:HB2	2.17	0.44
1:D:254:CYS:SG	1:D:319:ILE:HD11	2.58	0.43
1:A:230:TYR:O	1:A:286:CYS:HB2	2.17	0.43
1:C:39:LEU:HD13	1:C:253:ILE:CD1	2.48	0.43
1:A:50:VAL:HG22	1:A:198:MET:CE	2.49	0.43
1:D:311:ASN:HB2	1:D:319:ILE:HD12	2.00	0.43
2:H:637:ASP:HA	2:H:640:ARG:HG3	2.01	0.43
1:B:149:ASN:HB2	1:B:178:ARG:CZ	2.48	0.42
1:B:103:ASP:OD1	1:B:129:ARG:NH2	2.53	0.42
1:B:149:ASN:HB2	1:B:178:ARG:NE	2.35	0.42
2:E:635:ARG:CB	6:E:701:HOH:O	2.38	0.42
2:G:629:LEU:O	2:G:633:ALA:HB2	2.20	0.42
1:D:235:ALA:HB3	1:D:238:GLU:HG2	2.00	0.42
1:A:201:VAL:HG23	1:A:214:CYS:SG	2.60	0.42
1:A:75:SER:HB3	2:E:641:VAL:HG21	2.01	0.42
1:C:227:LEU:HD21	1:C:268:LEU:HB3	2.00	0.42
1:D:85:ILE:HA	1:D:88:MET:CE	2.47	0.42
1:B:145:GLU:HA	1:B:233:VAL:HG12	2.00	0.42
1:B:85:ILE:HA	1:B:88:MET:CE	2.50	0.42
1:B:281:SER:HA	1:B:282:PRO:HD3	1.78	0.42
1:D:54:LYS:HE2	1:D:60:GLY:O	2.19	0.42
1:A:270:LYS:HG2	3:A:401:GDP:C6	2.55	0.41
1:A:302:TYR:O	1:A:306:GLN:HG2	2.20	0.41
1:A:50:VAL:HA	1:A:198:MET:CE	2.49	0.41
1:D:36:LEU:CD2	1:D:220:ALA:HB3	2.50	0.41
1:C:78:ILE:HG22	1:C:82:ILE:CD1	2.51	0.41
1:C:270:LYS:HG2	3:C:401:GDP:C6	2.55	0.41
1:C:82:ILE:O	1:C:86:ARG:HG3	2.20	0.41
1:B:145:GLU:HA	1:B:233:VAL:HG11	2.02	0.40
1:D:312:LYS:HE2	4:D:407:SO4:O1	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:313:ARG:O	1:D:317:LYS:CB	2.69	0.40
1:B:85:ILE:HG13	1:B:88:MET:HE1	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	319/330 (97%)	301 (94%)	18 (6%)	0	100	100
1	B	313/330 (95%)	300 (96%)	13 (4%)	0	100	100
1	C	308/330 (93%)	294 (96%)	14 (4%)	0	100	100
1	D	323/330 (98%)	305 (94%)	18 (6%)	0	100	100
2	E	19/25 (76%)	16 (84%)	3 (16%)	0	100	100
2	F	20/25 (80%)	19 (95%)	1 (5%)	0	100	100
2	G	22/25 (88%)	19 (86%)	3 (14%)	0	100	100
2	H	20/25 (80%)	17 (85%)	3 (15%)	0	100	100
All	All	1344/1420 (95%)	1271 (95%)	73 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	272/285 (95%)	268 (98%)	4 (2%)	72	92
1	B	271/285 (95%)	260 (96%)	11 (4%)	37	73
1	C	275/285 (96%)	264 (96%)	11 (4%)	38	74
1	D	275/285 (96%)	266 (97%)	9 (3%)	45	80
2	E	19/24 (79%)	16 (84%)	3 (16%)	3	9
2	F	20/24 (83%)	17 (85%)	3 (15%)	3	11
2	G	21/24 (88%)	18 (86%)	3 (14%)	4	12
2	H	19/24 (79%)	19 (100%)	0	100	100
All	All	1172/1236 (95%)	1128 (96%)	44 (4%)	40	76

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	GLU
1	A	201	VAL
1	A	257	LYS
1	A	284	THR
1	B	85	ILE
1	B	90	ARG
1	B	100	ARG
1	B	160	ASP
1	B	179	VAL
1	B	201	VAL
1	B	206	SER
1	B	208	ARG
1	B	219	THR
1	B	233	VAL
1	B	348	LEU
1	C	63	GLU
1	C	160	ASP
1	C	171	GLN
1	C	201	VAL
1	C	206	SER
1	C	260	THR
1	C	261	ASP
1	C	281	SER
1	C	313	ARG
1	C	316	THR
1	C	345	LYS
1	D	75	SER

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Mol	Chain	Res	Type
1	D	160	ASP
1	D	166	ASN
1	D	186	GLU
1	D	242	ARG
1	D	313	ARG
1	D	317	LYS
1	D	319	ILE
1	D	353	LEU
2	E	629	LEU
2	E	641	VAL
2	E	642	LEU
2	F	634	LYS
2	F	641	VAL
2	F	642	LEU
2	G	630	ARG
2	G	641	VAL
2	G	645	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	79	GLN
1	B	68	GLN
1	B	79	GLN
1	D	166	ASN
1	D	306	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 ⓘ

25 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$
3	GDP	A	401	-	23,30,30	1.24	3 (13%)	30,47,47	1.73	7 (23%)
4	SO4	A	402	-	4,4,4	0.47	0	6,6,6	0.14	0
4	SO4	A	403	-	4,4,4	0.46	0	6,6,6	0.19	0
4	SO4	A	404	-	4,4,4	0.43	0	6,6,6	0.09	0
4	SO4	A	405	-	4,4,4	0.42	0	6,6,6	0.20	0
3	GDP	B	401	-	23,30,30	1.31	3 (13%)	30,47,47	1.83	7 (23%)
5	CIT	B	402	-	3,12,12	1.11	0	3,17,17	1.61	1 (33%)
5	CIT	B	403	-	3,12,12	0.98	0	3,17,17	1.99	1 (33%)
4	SO4	B	404	-	4,4,4	0.54	0	6,6,6	0.23	0
4	SO4	B	405	-	4,4,4	0.46	0	6,6,6	0.19	0
4	SO4	B	406	-	4,4,4	0.46	0	6,6,6	0.22	0
4	SO4	B	407	-	4,4,4	0.39	0	6,6,6	0.17	0
3	GDP	C	401	-	23,30,30	1.28	3 (13%)	30,47,47	1.79	7 (23%)
5	CIT	C	402	-	3,12,12	1.48	0	3,17,17	1.98	1 (33%)
4	SO4	C	403	-	4,4,4	0.45	0	6,6,6	0.08	0
4	SO4	C	404	-	4,4,4	0.41	0	6,6,6	0.25	0
4	SO4	C	405	-	4,4,4	0.46	0	6,6,6	0.11	0
4	SO4	C	406	-	4,4,4	0.40	0	6,6,6	0.25	0
3	GDP	D	401	-	23,30,30	1.21	3 (13%)	30,47,47	1.88	9 (30%)
5	CIT	D	402	-	3,12,12	1.87	1 (33%)	3,17,17	1.97	2 (66%)
4	SO4	D	403	-	4,4,4	0.55	0	6,6,6	0.28	0
4	SO4	D	404	-	4,4,4	0.44	0	6,6,6	0.09	0
4	SO4	D	405	-	4,4,4	0.38	0	6,6,6	0.13	0
4	SO4	D	406	-	4,4,4	0.49	0	6,6,6	0.14	0
4	SO4	D	407	-	4,4,4	0.39	0	6,6,6	0.07	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	GDP	A	401	-	-	0/12/32/32	0/3/3/3
4	SO4	A	402	-	-	0/0/0/0	0/0/0/0
4	SO4	A	403	-	-	0/0/0/0	0/0/0/0
4	SO4	A	404	-	-	0/0/0/0	0/0/0/0
4	SO4	A	405	-	-	0/0/0/0	0/0/0/0
3	GDP	B	401	-	-	0/12/32/32	0/3/3/3
5	CIT	B	402	-	-	0/6/16/16	0/0/0/0
5	CIT	B	403	-	-	0/6/16/16	0/0/0/0
4	SO4	B	404	-	-	0/0/0/0	0/0/0/0
4	SO4	B	405	-	-	0/0/0/0	0/0/0/0
4	SO4	B	406	-	-	0/0/0/0	0/0/0/0
4	SO4	B	407	-	-	0/0/0/0	0/0/0/0
3	GDP	C	401	-	-	0/12/32/32	0/3/3/3
5	CIT	C	402	-	-	0/6/16/16	0/0/0/0
4	SO4	C	403	-	-	0/0/0/0	0/0/0/0
4	SO4	C	404	-	-	0/0/0/0	0/0/0/0
4	SO4	C	405	-	-	0/0/0/0	0/0/0/0
4	SO4	C	406	-	-	0/0/0/0	0/0/0/0
3	GDP	D	401	-	-	0/12/32/32	0/3/3/3
5	CIT	D	402	-	-	0/6/16/16	0/0/0/0
4	SO4	D	403	-	-	0/0/0/0	0/0/0/0
4	SO4	D	404	-	-	0/0/0/0	0/0/0/0
4	SO4	D	405	-	-	0/0/0/0	0/0/0/0
4	SO4	D	406	-	-	0/0/0/0	0/0/0/0
4	SO4	D	407	-	-	0/0/0/0	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	402	CIT	C2-C3	-2.75	1.50	1.54
3	D	401	GDP	C5-C4	2.37	1.45	1.40
3	A	401	GDP	O4'-C1'	2.56	1.44	1.41
3	A	401	GDP	C5-C4	2.77	1.46	1.40
3	B	401	GDP	C5-C4	2.85	1.46	1.40
3	C	401	GDP	O4'-C1'	2.94	1.44	1.41
3	D	401	GDP	C6-C5	2.96	1.47	1.41
3	C	401	GDP	C5-C4	3.13	1.47	1.40
3	D	401	GDP	O4'-C1'	3.36	1.45	1.41
3	B	401	GDP	C6-C5	3.41	1.48	1.41
3	B	401	GDP	O4'-C1'	3.42	1.45	1.41
3	C	401	GDP	C6-C5	3.52	1.48	1.41
3	A	401	GDP	C6-C5	3.73	1.48	1.41

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	GDP	C5-C6-N1	-3.99	118.13	123.59
3	B	401	GDP	PA-O3A-PB	-3.92	119.52	132.67
3	B	401	GDP	C5-C6-N1	-3.88	118.28	123.59
3	A	401	GDP	C5-C6-N1	-3.83	118.34	123.59
3	D	401	GDP	C6-C5-C4	-3.83	116.32	120.90
3	D	401	GDP	PA-O3A-PB	-3.67	120.36	132.67
3	C	401	GDP	C6-C5-C4	-3.63	116.56	120.90
3	D	401	GDP	N3-C2-N1	-3.60	121.96	127.44
3	B	401	GDP	N3-C2-N1	-3.26	122.48	127.44
3	D	401	GDP	C5-C6-N1	-3.08	119.37	123.59
3	B	401	GDP	C6-C5-C4	-2.97	117.35	120.90
3	A	401	GDP	C4-C5-N7	-2.95	106.76	109.48
3	A	401	GDP	N3-C2-N1	-2.94	122.96	127.44
3	C	401	GDP	N3-C2-N1	-2.91	123.01	127.44
3	A	401	GDP	O4'-C1'-N9	-2.79	102.26	108.10
3	A	401	GDP	C6-C5-C4	-2.78	117.57	120.90
3	D	401	GDP	O3'-C3'-C4'	-2.70	102.94	111.05
3	C	401	GDP	C4-C5-N7	-2.38	107.29	109.48
3	A	401	GDP	PA-O3A-PB	-2.29	124.97	132.67
3	D	401	GDP	C1'-N9-C4	-2.22	123.60	126.94
3	B	401	GDP	C4-C5-N7	-2.10	107.54	109.48
3	C	401	GDP	C1'-N9-C4	-2.10	123.77	126.94
3	C	401	GDP	PA-O3A-PB	-2.01	125.92	132.67
5	D	402	CIT	C4-C3-C2	2.05	114.71	109.81
3	B	401	GDP	N2-C2-N1	2.10	120.68	117.20
3	D	401	GDP	O3B-PB-O2B	2.27	116.00	107.38
5	C	402	CIT	C3-C4-C5	2.45	118.87	114.96
5	D	402	CIT	C3-C4-C5	2.65	119.19	114.96
3	D	401	GDP	N2-C2-N1	2.69	121.65	117.20
5	B	402	CIT	C3-C4-C5	2.76	119.36	114.96
5	B	403	CIT	C4-C3-C2	3.39	117.91	109.81
3	D	401	GDP	C6-N1-C2	3.81	121.22	115.94
3	A	401	GDP	C6-N1-C2	3.87	121.31	115.94
3	B	401	GDP	C6-N1-C2	4.12	121.66	115.94
3	C	401	GDP	C6-N1-C2	4.57	122.28	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	GDP	1	0
5	B	402	CIT	1	0
3	C	401	GDP	1	0
5	C	402	CIT	3	0
4	C	406	SO4	1	0
4	D	407	SO4	1	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	320/330 (96%)	-0.19	3 (0%) 85 84	35, 60, 100, 125	0
1	B	316/330 (95%)	-0.23	7 (2%) 65 60	37, 57, 91, 125	0
1	C	316/330 (95%)	-0.10	10 (3%) 51 43	36, 62, 110, 145	0
1	D	324/330 (98%)	-0.10	12 (3%) 45 38	34, 61, 103, 143	0
2	E	21/25 (84%)	-0.07	0 100 100	59, 69, 85, 87	0
2	F	22/25 (88%)	-0.13	0 100 100	50, 63, 84, 90	0
2	G	24/25 (96%)	0.10	2 (8%) 14 9	52, 64, 109, 127	0
2	H	22/25 (88%)	0.36	1 (4%) 37 31	64, 79, 109, 128	0
All	All	1365/1420 (96%)	-0.14	35 (2%) 59 54	34, 62, 104, 145	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	116	GLU	5.0
1	D	117	GLY	4.9
1	D	204	GLN	4.7
1	B	98	SER	4.3
1	D	316	THR	4.3
1	D	206	SER	3.8
2	G	622	GLU	3.7
1	D	118	PHE	3.6
1	C	204	GLN	3.6
1	C	147	GLN	3.2
1	B	203	GLY	3.0
1	C	107	LEU	2.9
1	C	118	PHE	2.9
1	C	119	MET	2.9
1	A	350	ASP	2.9
1	D	350	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	203	GLY	2.7
1	B	207	GLU	2.6
1	D	147	GLN	2.6
1	D	107	LEU	2.5
1	B	193	ASP	2.5
1	A	141	ASN	2.4
1	A	147	GLN	2.4
1	B	118	PHE	2.4
2	H	622	GLU	2.4
1	D	205	ARG	2.3
1	B	134	SER	2.3
1	D	211	TRP	2.2
2	G	643	LEU	2.2
1	C	106	GLN	2.1
1	B	97	ASP	2.1
1	C	97	ASP	2.1
1	C	98	SER	2.0
1	C	207	GLU	2.0
1	C	124	ALA	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, 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(Å ²)	Q<0.9
5	CIT	C	402	13/13	0.90	0.25	5.55	47,60,72,76	0
4	SO4	B	406	5/5	0.75	0.25	3.41	130,135,139,146	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	GDP	A	401	28/28	0.97	0.18	0.81	48,54,58,59	0
5	CIT	B	403	13/13	0.96	0.17	0.29	56,58,64,67	0
5	CIT	B	402	13/13	0.95	0.17	-0.04	56,59,67,72	0
3	GDP	C	401	28/28	0.99	0.15	-0.23	44,49,51,52	0
4	SO4	A	404	5/5	0.95	0.15	-0.27	107,108,116,120	0
3	GDP	D	401	28/28	0.99	0.15	-0.28	38,43,47,48	0
3	GDP	B	401	28/28	0.99	0.16	-0.49	37,42,47,48	0
4	SO4	C	403	5/5	0.90	0.14	-0.67	103,108,113,113	0
5	CIT	D	402	13/13	0.96	0.15	-0.98	42,47,53,57	0
4	SO4	B	404	5/5	0.88	0.19	-	97,110,116,117	0
4	SO4	A	405	5/5	0.91	0.22	-	107,112,115,124	0
4	SO4	C	404	5/5	0.90	0.21	-	115,120,123,123	0
4	SO4	B	405	5/5	0.81	0.26	-	116,120,127,130	0
4	SO4	B	407	5/5	0.90	0.38	-	134,138,141,142	0
4	SO4	D	406	5/5	0.78	0.32	-	119,124,132,132	0
4	SO4	D	405	5/5	0.81	0.30	-	153,158,160,161	0
4	SO4	C	406	5/5	0.92	0.16	-	126,130,130,133	0
4	SO4	D	404	5/5	0.92	0.28	-	122,131,137,138	0
4	SO4	C	405	5/5	0.82	0.32	-	128,133,138,141	0
4	SO4	D	403	5/5	0.95	0.15	-	91,96,100,101	0
4	SO4	A	402	5/5	0.85	0.17	-	110,115,123,126	0
4	SO4	A	403	5/5	0.92	0.14	-	110,111,115,115	0
4	SO4	D	407	5/5	0.94	0.28	-	131,133,135,136	0

6.5 Other polymers [i](#)

There are no such residues in this entry.