



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:34 PM GMT

PDB ID : 3W0L
Title : The crystal structure of Xenopus Glucokinase and Glucokinase Regulatory Protein complex
Authors : Choi, J.M.; Seo, M.H.; Kyeong, H.H.; Kim, E.; Kim, H.S.
Deposited on : 2012-10-31
Resolution : 2.92 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>

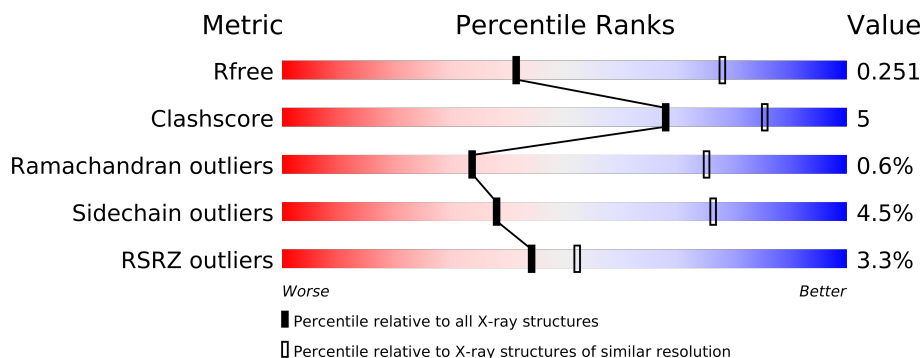
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.92 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	1172 (2.94-2.90)
Clashscore	79885	1461 (2.94-2.90)
Ramachandran outliers	78287	1419 (2.94-2.90)
Sidechain outliers	78261	1421 (2.94-2.90)
RSRZ outliers	66119	1173 (2.94-2.90)

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. 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	458	
1	C	458	
2	B	619	
2	D	619	

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

Mol	Type	Chain	Res	Geometry	Electron density
3	SO4	B	702	-	X
3	SO4	B	703	-	X
5	F6R	D	701	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15800 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 Glucokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	426	Total	C	N	O	S	0	0	0
			3319	2075	564	648	32			
1	C	407	Total	C	N	O	S	0	0	0
			3175	1988	540	616	31			

- Molecule 2 is a protein called Glucokinase regulatory protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	598	Total	C	N	O	S	0	0	0
			4668	2946	806	894	22			
2	D	577	Total	C	N	O	S	0	0	0
			4499	2846	776	856	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	530	GLN	HIS	SEE REMARK 999	UNP Q91754
D	530	GLN	HIS	SEE REMARK 999	UNP Q91754

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

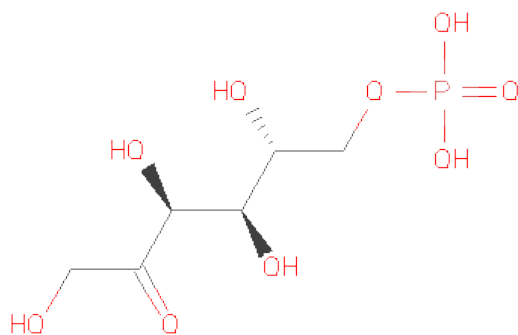


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		
4	C	1	Total	Na	0	0
			1	1		

- Molecule 5 is FRUCTOSE -6-PHOSPHATE (three-letter code: F6R) (formula: C₆H₁₃O₉P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	O	P	0	0
			16	6	9	1		
5	D	1	Total	C	O	P	0	0
			16	6	9	1		

- Molecule 6 is water.

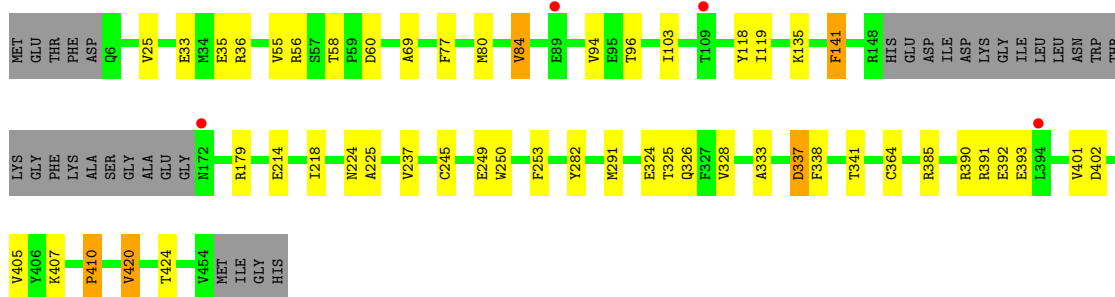
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	32	Total	O	0	0
			32	32		
6	B	26	Total	O	0	0
			26	26		
6	C	15	Total	O	0	0
			15	15		
6	D	12	Total	O	0	0
			12	12		

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.

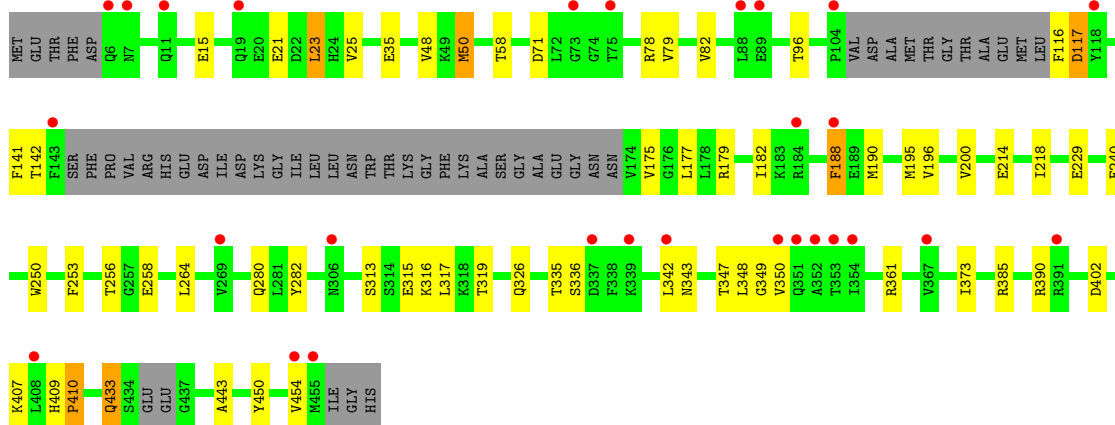
• Molecule 1: Glucokinase

Chain A: 



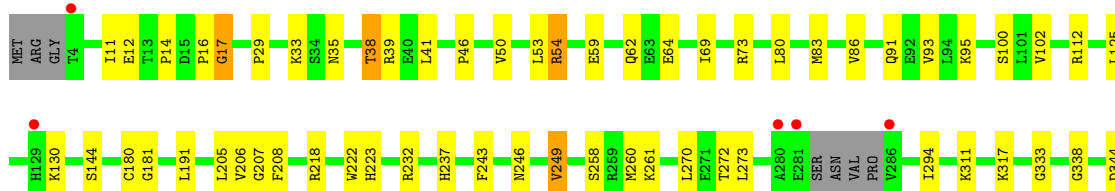
• Molecule 1: Glucokinase

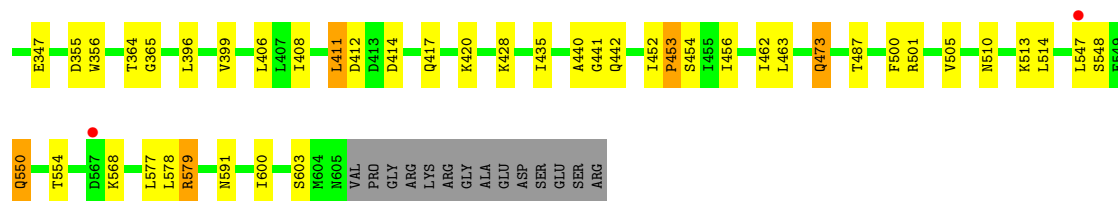
Chain C: 



• Molecule 2: Glucokinase regulatory protein

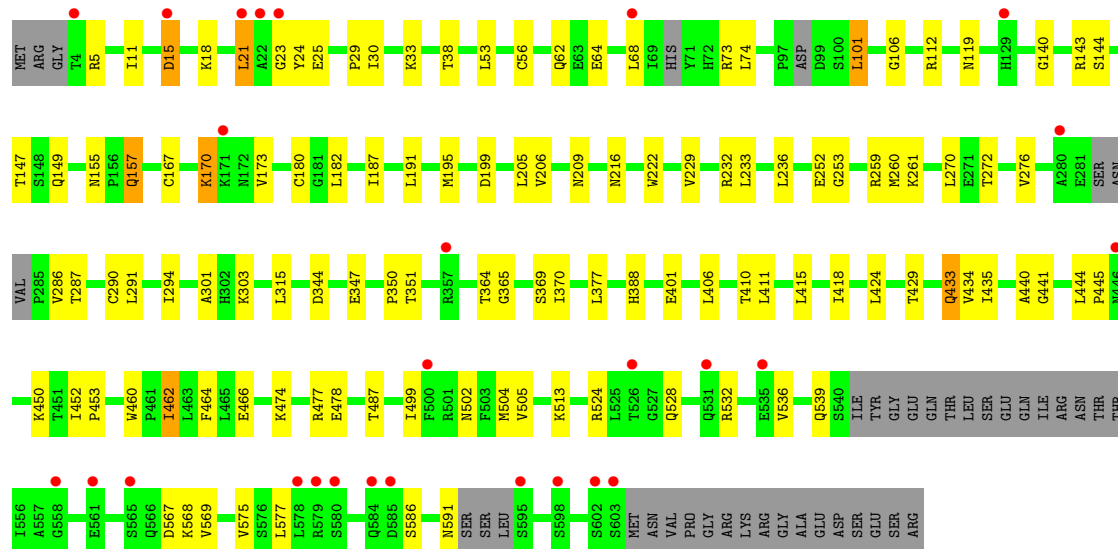
Chain B: 





• Molecule 2: Glucokinase regulatory protein

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	109.32Å 130.03Å 175.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.48 – 2.92 28.48 – 2.92	Depositor EDS
% Data completeness (in resolution range)	97.3 (28.48-2.92) 88.8 (28.48-2.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.64 (at 2.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.242 , 0.277 0.213 , 0.251	Depositor DCC
R_{free} test set	2439 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	49.6	Xtriage
Anisotropy	0.739	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 13.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 53519 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	15800	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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: NA, SO4, F6R

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	0.21	0/3367	0.35	0/4532
1	C	0.21	0/3219	0.35	0/4327
2	B	0.21	0/4748	0.38	0/6419
2	D	0.21	0/4574	0.37	0/6177
All	All	0.21	0/15908	0.37	0/21455

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	3319	0	3270	24	0
1	C	3175	0	3135	26	0
2	B	4668	0	4718	53	0
2	D	4499	0	4557	54	0
3	A	5	0	0	0	0
3	B	10	0	0	0	0
3	C	5	0	0	0	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	1	0	0	0	0
5	B	16	0	11	1	0
5	D	16	0	11	2	0
6	A	32	0	0	0	0
6	B	26	0	0	0	0
6	C	15	0	0	0	0
6	D	12	0	0	0	0
All	All	15800	0	15702	155	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 5.

All (155) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:513:LYS:NZ	5:B:701:F6R:O5	2.21	0.74
2:D:101:LEU:HD22	2:D:170:LYS:HG2	1.73	0.71
2:D:112:ARG:NH1	2:D:144:SER:O	2.28	0.67
2:D:21:LEU:HD13	2:D:23:GLY:H	1.59	0.66
2:B:112:ARG:NH1	2:B:144:SER:O	2.29	0.65
2:B:11:ILE:HD11	2:B:54:ARG:HH12	1.62	0.65
1:C:71:ASP:HB3	1:C:78:ARG:HB3	1.77	0.65
2:D:536:VAL:HG11	2:D:577:LEU:HB2	1.80	0.63
2:B:311:LYS:HB3	2:B:456:ILE:HG12	1.80	0.63
2:B:38:THR:O	2:B:38:THR:OG1	2.13	0.63
2:D:434:VAL:HG21	2:D:452:ILE:HD13	1.81	0.63
1:C:316:LYS:HG3	1:C:348:LEU:HB3	1.81	0.63
2:B:93:VAL:HG11	2:B:102:VAL:HG23	1.81	0.62
1:A:58:THR:OG1	1:A:60:ASP:OD1	2.15	0.62
1:C:23:LEU:HD21	1:C:373:ILE:HB	1.82	0.62
2:B:53:LEU:HD12	2:B:487:THR:HG23	1.82	0.61
1:C:196:VAL:HG13	1:C:200:VAL:HB	1.83	0.61
1:C:315:GLU:O	1:C:319:THR:OG1	2.19	0.60
1:C:229:GLU:OE1	1:C:385:ARG:NH1	2.34	0.60
2:D:64:GLU:HA	2:D:73:ARG:HG3	1.83	0.60
1:A:324:GLU:OE1	1:A:326:GLN:NE2	2.32	0.60
2:D:444:LEU:HD12	2:D:445:PRO:HD2	1.83	0.60
2:D:233:LEU:HA	2:D:236:LEU:HD12	1.82	0.60
2:B:568:LYS:NZ	2:B:591:ASN:OD1	2.35	0.59
1:A:337:ASP:N	1:A:337:ASP:OD2	2.35	0.59
2:B:180:CYS:O	2:B:208:PHE:N	2.35	0.59
1:A:402:ASP:OD2	1:A:407:LYS:NZ	2.28	0.59
2:D:568:LYS:NZ	2:D:591:ASN:OD1	2.35	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:214:GLU:OE1	1:A:390:ARG:NH1	2.33	0.59
1:A:56:ARG:NH2	1:A:135:LYS:O	2.35	0.58
2:D:567:ASP:OD2	2:D:568:LYS:N	2.36	0.58
2:D:575:VAL:HG13	2:D:586:SER:HB3	1.85	0.58
1:C:48:VAL:HG12	1:C:50:MET:HG2	1.86	0.58
2:D:62:GLN:OE1	2:D:73:ARG:NH1	2.37	0.57
2:D:539:GLN:NE2	2:D:569:VAL:O	2.37	0.57
2:D:513:LYS:NZ	5:D:701:F6R:O5	2.32	0.57
2:B:206:VAL:HG21	2:B:270:LEU:HD21	1.86	0.57
2:B:80:LEU:HD23	2:B:83:MET:HE3	1.87	0.56
2:B:505:VAL:HG11	2:B:600:ILE:HD11	1.88	0.56
2:D:53:LEU:HD12	2:D:487:THR:HG23	1.88	0.56
2:D:474:LYS:NZ	2:D:478:GLU:OE2	2.39	0.56
2:B:414:ASP:HB3	2:B:417:GLN:HG2	1.88	0.56
1:A:77:PHE:HB2	1:A:103:ILE:HD11	1.88	0.55
2:B:14:PRO:O	2:B:62:GLN:NE2	2.40	0.54
2:D:253:GLY:O	2:D:502:ASN:ND2	2.41	0.53
2:B:86:VAL:HB	2:B:273:LEU:HD11	1.91	0.53
1:C:117:ASP:OD1	1:C:117:ASP:N	2.37	0.53
1:A:35:GLU:HG2	1:A:385:ARG:HH12	1.74	0.52
1:C:175:VAL:HG22	1:C:195:MET:HG3	1.92	0.52
1:C:343:ASN:O	1:C:347:THR:OG1	2.23	0.52
2:D:15:ASP:N	2:D:15:ASP:OD2	2.41	0.52
2:D:25:GLU:O	2:D:33:LYS:NZ	2.43	0.52
2:B:463:LEU:HD12	2:B:473:GLN:HG2	1.92	0.51
2:B:93:VAL:HG13	2:B:100:SER:HB3	1.93	0.51
1:C:313:SER:HB3	1:C:317:LEU:HB3	1.91	0.51
2:B:579:ARG:NH1	2:B:603:SER:OG	2.44	0.51
1:C:407:LYS:HE2	1:C:433:GLN:HG3	1.92	0.51
2:D:191:LEU:HD11	2:D:205:LEU:HD13	1.92	0.51
2:D:347:GLU:O	2:D:351:THR:OG1	2.26	0.51
1:C:142:THR:HG21	1:C:443:ALA:H	1.75	0.51
2:B:218:ARG:NE	2:B:223:HIS:O	2.44	0.51
2:B:180:CYS:N	2:B:181:GLY:HA3	2.25	0.50
2:D:406:LEU:HD11	2:D:435:ILE:HG13	1.94	0.50
2:B:411:LEU:HD23	2:B:442:GLN:HG3	1.92	0.50
1:C:218:ILE:HG12	1:C:402:ASP:HB3	1.93	0.50
2:B:59:GLU:O	2:B:73:ARG:NH2	2.45	0.50
2:B:249:VAL:HG13	2:B:261:LYS:HE2	1.94	0.49
2:B:510:ASN:H	2:B:514:LEU:HD12	1.78	0.49
1:A:33:GLU:OE2	1:A:36:ARG:NH1	2.45	0.49
1:C:182:ILE:HG23	1:C:188:PHE:HB3	1.94	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:287:THR:HG23	2:D:290:CYS:H	1.78	0.48
1:A:84:VAL:HG12	1:A:94:VAL:HG23	1.94	0.48
1:C:82:VAL:HG22	1:C:96:THR:HG22	1.95	0.48
2:B:112:ARG:NH2	2:B:347:GLU:OE1	2.46	0.48
1:C:179:ARG:NH1	1:C:190:MET:O	2.46	0.48
2:B:272:THR:HG23	2:B:294:ILE:HB	1.94	0.48
2:D:112:ARG:NH2	2:D:347:GLU:OE1	2.46	0.48
2:D:276:VAL:HG21	2:D:291:LEU:HD23	1.96	0.47
1:A:333:ALA:HB2	1:A:410:PRO:HG2	1.94	0.47
2:D:182:LEU:HD13	2:D:209:ASN:HB2	1.97	0.47
2:D:206:VAL:HG21	2:D:270:LEU:HD21	1.97	0.47
2:B:64:GLU:HB3	2:B:73:ARG:HG2	1.97	0.47
2:B:191:LEU:HD11	2:B:205:LEU:HD13	1.97	0.47
2:D:462:ILE:HD11	2:D:464:PHE:CZ	2.50	0.47
1:C:214:GLU:OE1	1:C:390:ARG:NH2	2.32	0.47
2:D:440:ALA:HA	2:D:441:GLY:HA2	1.56	0.46
2:D:106:GLY:HA2	2:D:187:ILE:HD11	1.98	0.46
2:D:315:LEU:HD13	2:D:433:GLN:HG2	1.97	0.46
2:B:399:VAL:HG22	2:B:428:LYS:HB3	1.96	0.46
2:D:119:ASN:ND2	2:D:370:ILE:O	2.48	0.46
1:A:179:ARG:NH2	2:B:412:ASP:OD1	2.46	0.46
1:C:256:THR:OG1	1:C:258:GLU:OE1	2.25	0.46
2:D:167:CYS:HB3	2:D:173:VAL:HG21	1.98	0.46
2:B:333:GLY:HA3	2:B:338:GLY:HA2	1.98	0.45
1:C:253:PHE:O	1:C:282:TYR:HB2	2.17	0.45
2:D:415:LEU:HD23	2:D:418:ILE:HD12	1.98	0.45
1:C:409:HIS:HA	1:C:410:PRO:HD3	1.79	0.45
1:C:15:GLU:HG2	1:C:264:LEU:HD22	1.98	0.45
1:A:119:ILE:HG21	1:A:141:PHE:HZ	1.82	0.45
2:D:536:VAL:HG21	2:D:577:LEU:HD13	1.99	0.45
2:B:46:PRO:HG3	2:B:317:LYS:HE2	1.99	0.44
2:D:38:THR:OG1	2:D:502:ASN:ND2	2.50	0.44
2:D:180:CYS:N	5:D:701:F6R:O1P	2.51	0.44
2:D:229:VAL:HA	2:D:232:ARG:HD2	1.99	0.44
2:D:155:ASN:OD1	2:D:157:GLN:NE2	2.50	0.44
1:C:335:THR:OG1	1:C:336:SER:N	2.51	0.44
2:D:272:THR:HG23	2:D:294:ILE:HB	2.00	0.43
1:A:291:MET:HB3	1:A:325:THR:HG23	2.00	0.43
2:D:364:THR:HA	2:D:365:GLY:HA2	1.53	0.43
2:B:440:ALA:HA	2:B:441:GLY:HA2	1.50	0.43
2:B:364:THR:HA	2:B:365:GLY:HA2	1.63	0.43
2:B:50:VAL:O	2:B:54:ARG:HB3	2.19	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:550:GLN:O	2:B:554:THR:OG1	2.37	0.43
2:D:252:GLU:HA	2:D:261:LYS:HD3	2.01	0.43
2:B:91:GLN:O	2:B:95:LYS:HG3	2.18	0.43
2:D:365:GLY:N	2:D:369:SER:OG	2.47	0.42
2:D:29:PRO:O	2:D:33:LYS:HG3	2.19	0.42
1:A:69:ALA:HB3	1:A:80:MET:HB3	2.00	0.42
2:B:452:ILE:HA	2:B:453:PRO:HD3	1.93	0.42
1:C:78:ARG:NH2	1:C:450:TYR:OH	2.53	0.42
2:B:406:LEU:HD11	2:B:435:ILE:HG13	2.00	0.42
2:B:35:ASN:HB3	2:B:38:THR:HG23	2.01	0.42
2:D:301:ALA:HA	2:D:460:TRP:HZ3	1.84	0.42
2:B:237:HIS:ND1	2:B:243:PHE:HA	2.35	0.42
2:D:143:ARG:O	2:D:147:THR:HG22	2.20	0.42
2:D:25:GLU:OE2	2:D:524:ARG:NH1	2.52	0.42
1:A:237:VAL:HG22	2:B:462:ILE:HB	2.01	0.42
2:B:16:PRO:HA	2:B:17:GLY:HA3	1.81	0.42
1:A:103:ILE:HD13	1:A:118:TYR:HE2	1.85	0.42
2:D:30:ILE:HA	2:D:33:LYS:HD2	2.02	0.42
2:B:125:LEU:HB3	2:B:130:LYS:HB2	2.01	0.42
2:B:500:PHE:CD2	2:B:501:ARG:HG3	2.55	0.42
2:B:411:LEU:HD12	2:B:411:LEU:HA	1.86	0.41
2:B:207:GLY:O	2:B:246:ASN:HA	2.20	0.41
2:D:11:ILE:HG22	2:D:303:LYS:HB2	2.02	0.41
2:D:24:TYR:O	2:D:33:LYS:NZ	2.46	0.41
2:D:401:GLU:HG2	2:D:429:THR:HA	2.02	0.41
1:C:35:GLU:OE1	1:C:385:ARG:NH2	2.41	0.41
1:C:21:GLU:O	1:C:25:VAL:HG23	2.21	0.41
2:B:408:ILE:HG13	2:B:435:ILE:HB	2.03	0.41
1:A:55:VAL:HB	1:A:245:CYS:HB3	2.03	0.41
1:A:218:ILE:HG12	1:A:402:ASP:HB3	2.01	0.41
1:A:328:VAL:HG13	1:A:364:CYS:HB3	2.01	0.41
2:B:29:PRO:O	2:B:33:LYS:HG3	2.21	0.41
2:B:578:LEU:HA	2:B:578:LEU:HD12	1.84	0.41
2:D:450:LYS:HB2	2:D:450:LYS:HE3	1.96	0.41
1:A:420:VAL:O	1:A:424:THR:N	2.54	0.41
1:A:338:PHE:HB3	1:A:341:THR:HB	2.03	0.41
2:B:355:ASP:OD1	2:B:356:TRP:N	2.54	0.41
2:B:180:CYS:SG	2:B:258:SER:HB2	2.61	0.40
1:A:253:PHE:O	1:A:282:TYR:HB2	2.20	0.40
2:D:56:CYS:HB3	2:D:261:LYS:HD2	2.03	0.40
1:A:224:ASN:OD1	1:A:225:ALA:N	2.51	0.40
2:B:453:PRO:HB2	2:B:454:SER:H	1.70	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:147:THR:HG23	2:D:149:GLN:HG2	2.03	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	422/458 (92%)	410 (97%)	11 (3%)	1 (0%)	56	89
1	C	399/458 (87%)	373 (94%)	23 (6%)	3 (1%)	27	67
2	B	594/619 (96%)	556 (94%)	34 (6%)	4 (1%)	30	72
2	D	565/619 (91%)	527 (93%)	34 (6%)	4 (1%)	30	72
All	All	1980/2154 (92%)	1866 (94%)	102 (5%)	12 (1%)	33	75

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	453	PRO
2	D	453	PRO
2	B	548	SER
1	A	410	PRO
1	C	454	VAL
2	D	260	MET
1	C	410	PRO
2	D	350	PRO
2	D	140	GLY
2	B	69	ILE
2	B	17	GLY
1	C	349	GLY

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	363/388 (94%)	350 (96%)	13 (4%)	47	84
1	C	347/388 (89%)	330 (95%)	17 (5%)	35	73
2	B	524/541 (97%)	506 (97%)	18 (3%)	49	85
2	D	504/541 (93%)	474 (94%)	30 (6%)	27	62
All	All	1738/1858 (94%)	1660 (96%)	78 (4%)	38	76

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	VAL
1	A	84	VAL
1	A	96	THR
1	A	141	PHE
1	A	249	GLU
1	A	250	TRP
1	A	337	ASP
1	A	391	ARG
1	A	392	GLU
1	A	393	GLU
1	A	401	VAL
1	A	405	VAL
1	A	420	VAL
2	B	12	GLU
2	B	38	THR
2	B	39	ARG
2	B	41	LEU
2	B	54	ARG
2	B	222	TRP
2	B	232	ARG
2	B	249	VAL
2	B	260	MET
2	B	344	ASP
2	B	396	LEU
2	B	411	LEU
2	B	420	LYS

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Mol	Chain	Res	Type
2	B	473	GLN
2	B	547	LEU
2	B	550	GLN
2	B	577	LEU
2	B	579	ARG
1	C	23	LEU
1	C	50	MET
1	C	58	THR
1	C	79	VAL
1	C	116	PHE
1	C	117	ASP
1	C	141	PHE
1	C	177	LEU
1	C	188	PHE
1	C	240	GLU
1	C	250	TRP
1	C	280	GLN
1	C	326	GLN
1	C	342	LEU
1	C	350	VAL
1	C	361	ARG
1	C	433	GLN
2	D	5	ARG
2	D	15	ASP
2	D	18	LYS
2	D	21	LEU
2	D	68	LEU
2	D	74	LEU
2	D	101	LEU
2	D	157	GLN
2	D	170	LYS
2	D	195	MET
2	D	199	ASP
2	D	216	ASN
2	D	222	TRP
2	D	259	ARG
2	D	286	VAL
2	D	344	ASP
2	D	377	LEU
2	D	388	HIS
2	D	410	THR
2	D	411	LEU

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Mol	Chain	Res	Type
2	D	424	LEU
2	D	433	GLN
2	D	462	ILE
2	D	466	GLU
2	D	477	ARG
2	D	499	ILE
2	D	504	MET
2	D	505	VAL
2	D	528	GLN
2	D	532	ARG

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

Mol	Chain	Res	Type
2	B	149	GLN
2	B	473	GLN
2	D	157	GLN
2	D	502	ASN

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 ⓘ

Of 8 ligands modelled in this entry, 2 are 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	SO4	A	501	-	4,4,4	0.21	0	6,6,6	0.06	0
5	F6R	B	701	-	15,15,15	1.39	2 (13%)	21,21,21	1.34	3 (14%)
3	SO4	B	702	-	4,4,4	0.21	0	6,6,6	0.07	0
3	SO4	B	703	-	4,4,4	0.22	0	6,6,6	0.07	0
3	SO4	C	501	-	4,4,4	0.19	0	6,6,6	0.09	0
5	F6R	D	701	-	15,15,15	1.31	2 (13%)	21,21,21	1.32	4 (19%)

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	SO4	A	501	-	-	0/0/0/0	0/0/0/0
5	F6R	B	701	-	-	0/20/20/20	0/0/0/0
3	SO4	B	702	-	-	0/0/0/0	0/0/0/0
3	SO4	B	703	-	-	0/0/0/0	0/0/0/0
3	SO4	C	501	-	-	0/0/0/0	0/0/0/0
5	F6R	D	701	-	-	0/20/20/20	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	701	F6R	O5-C5	-2.33	1.38	1.43
5	D	701	F6R	O5-C5	-2.21	1.38	1.43
5	D	701	F6R	C3-C2	-2.05	1.49	1.52
5	B	701	F6R	C6-C5	-2.03	1.48	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	701	F6R	C1-C2-C3	3.10	122.12	116.26
5	D	701	F6R	C1-C2-C3	3.01	121.96	116.26
5	D	701	F6R	C4-C3-C2	-2.46	107.58	110.77
5	B	701	F6R	O3-C3-C2	-2.44	107.18	111.16
5	D	701	F6R	O3-C3-C2	-2.24	107.50	111.16
5	B	701	F6R	C4-C3-C2	-2.15	107.98	110.77
5	D	701	F6R	O4-C4-C5	2.03	113.88	108.74

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	426/458 (93%)	-0.07	4 (0%) 81 87	24, 44, 73, 96	0
1	C	407/458 (88%)	0.31	28 (6%) 17 20	27, 55, 105, 126	0
2	B	598/619 (96%)	-0.12	7 (1%) 75 83	25, 44, 72, 97	0
2	D	577/619 (93%)	0.28	27 (4%) 30 37	26, 59, 103, 127	0
All	All	2008/2154 (93%)	0.10	66 (3%) 44 52	24, 50, 95, 127	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	104	PRO	5.1
1	C	7	ASN	4.8
2	D	68	LEU	4.5
2	B	4	THR	4.4
1	C	351	GLN	4.1
1	C	11	GLN	4.0
2	D	22	ALA	3.6
2	D	280	ALA	3.6
2	D	357	ARG	3.6
2	D	531	GLN	3.5
2	D	21	LEU	3.5
2	D	171	LYS	3.4
1	C	6	GLN	3.1
2	D	585	ASP	3.0
1	C	455	MET	3.0
1	A	172	ASN	2.9
2	D	595	SER	2.9
1	C	342	LEU	2.9
1	C	306	ASN	2.9
2	D	526	THR	2.8
2	D	584	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	603	SER	2.8
2	D	598	SER	2.7
1	C	367	VAL	2.7
2	D	565	SER	2.7
2	D	15	ASP	2.7
2	D	579	ARG	2.6
1	C	89	GLU	2.6
2	D	558	GLY	2.6
2	B	567	ASP	2.6
1	C	75	THR	2.6
2	D	580	SER	2.5
2	D	578	LEU	2.5
2	D	23	GLY	2.5
1	C	88	LEU	2.5
1	C	408	LEU	2.5
2	D	602	SER	2.5
1	C	269	VAL	2.4
1	C	118	TYR	2.4
1	C	350	VAL	2.4
1	C	353	THR	2.4
1	A	394	LEU	2.4
1	C	352	ALA	2.4
2	B	280	ALA	2.4
2	B	281	GLU	2.3
1	A	109	THR	2.3
1	C	391	ARG	2.3
1	C	354	ILE	2.3
2	D	446	ASN	2.3
1	A	89	GLU	2.3
1	C	19	GLN	2.2
1	C	339	LYS	2.2
1	C	143	PHE	2.2
2	B	286	VAL	2.2
1	C	337	ASP	2.2
2	B	547	LEU	2.1
2	D	500	PHE	2.1
2	D	561	GLU	2.1
2	D	129	HIS	2.1
2	B	129	HIS	2.1
2	D	535	GLU	2.1
1	C	454	VAL	2.0
2	D	4	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	184	ARG	2.0
1	C	188	PHE	2.0
1	C	73	GLY	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
3	SO4	B	703	5/5	0.34	4.24	75,81,103,116	0
5	F6R	D	701	16/16	0.33	3.31	55,94,102,102	0
3	SO4	B	702	5/5	0.36	2.52	71,72,92,96	0
5	F6R	B	701	16/16	0.23	1.97	36,66,70,72	0
3	SO4	C	501	5/5	0.12	-1.14	37,49,63,68	0
3	SO4	A	501	5/5	0.08	-1.82	36,42,55,68	0
4	NA	C	502	1/1	0.08	-2.07	39,39,39,39	0
4	NA	A	502	1/1	0.07	-2.13	42,42,42,42	0

6.5 Other polymers ⓘ

There are no such residues in this entry.