



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:38 PM UTC

PDB ID : 2GIX / pdb_00002gix
Title : Cytoplasmic Domain Structure of Kir2.1 containing Andersen's Mutation R218Q and Rescue Mutation T309K
Authors : Pegan, S.; Arrabit, C.; Slesinger, P.A.; Choe, S.
Deposited on : 2006-03-29
Resolution : 2.02 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

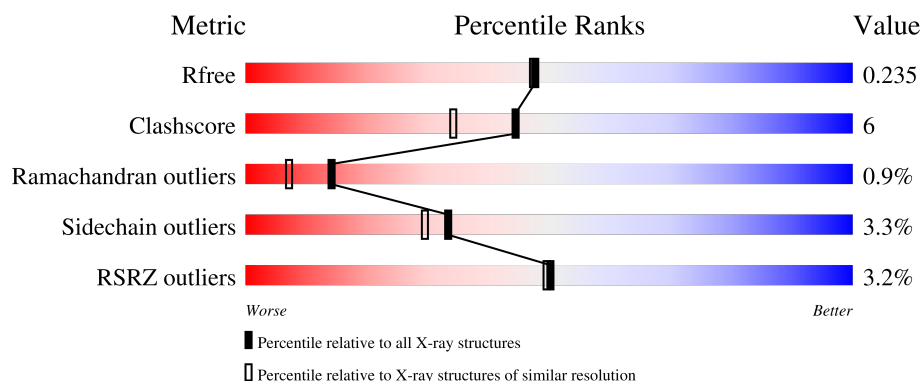
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

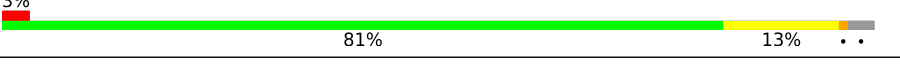
The reported resolution of this entry is 2.02 Å.

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	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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	208	
1	B	208	
1	C	208	
1	D	208	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7303 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 Inward rectifier potassium channel 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	0	0
			1654	1050	286	310	8			
1	B	201	Total	C	N	O	S	0	0	0
			1612	1022	280	302	8			
1	C	206	Total	C	N	O	S	0	0	0
			1654	1050	286	310	8			
1	D	205	Total	C	N	O	S	0	0	0
			1650	1049	285	308	8			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	218	GLN	ARG	engineered mutation	UNP P35561
A	309	LYS	THR	engineered mutation	UNP P35561
B	218	GLN	ARG	engineered mutation	UNP P35561
B	309	LYS	THR	engineered mutation	UNP P35561
C	218	GLN	ARG	engineered mutation	UNP P35561
C	309	LYS	THR	engineered mutation	UNP P35561
D	218	GLN	ARG	engineered mutation	UNP P35561
D	309	LYS	THR	engineered mutation	UNP P35561
A	40	GLY	-	cloning artifact	UNP P35561
A	41	SER	-	cloning artifact	UNP P35561
A	42	HIS	-	cloning artifact	UNP P35561
A	43	GLY	-	cloning artifact	UNP P35561
B	40	GLY	-	cloning artifact	UNP P35561
B	41	SER	-	cloning artifact	UNP P35561
B	42	HIS	-	cloning artifact	UNP P35561
B	43	GLY	-	cloning artifact	UNP P35561
C	40	GLY	-	cloning artifact	UNP P35561
C	41	SER	-	cloning artifact	UNP P35561
C	42	HIS	-	cloning artifact	UNP P35561
C	43	GLY	-	cloning artifact	UNP P35561
D	40	GLY	-	cloning artifact	UNP P35561

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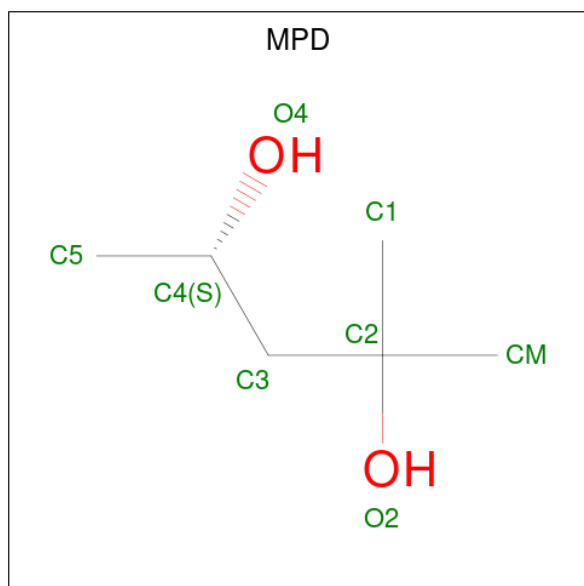
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Chain	Residue	Modelled	Actual	Comment	Reference
D	41	SER	-	cloning artifact	UNP P35561
D	42	HIS	-	cloning artifact	UNP P35561
D	43	GLY	-	cloning artifact	UNP P35561

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 8 6 2	0	0
3	B	1	Total C O 8 6 2	0	0
3	C	1	Total C O 8 6 2	0	0
3	D	1	Total C O 8 6 2	0	0

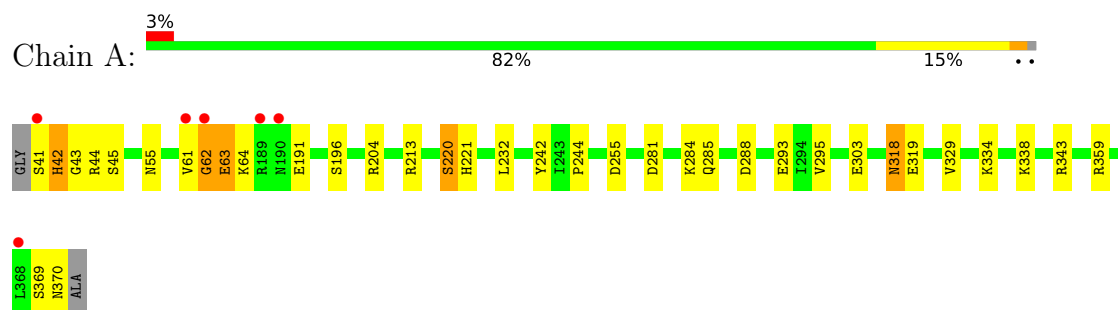
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	192	Total 192	O 192	0	0
4	B	169	Total 169	O 169	0	0
4	C	164	Total 164	O 164	0	0
4	D	175	Total 175	O 175	0	0

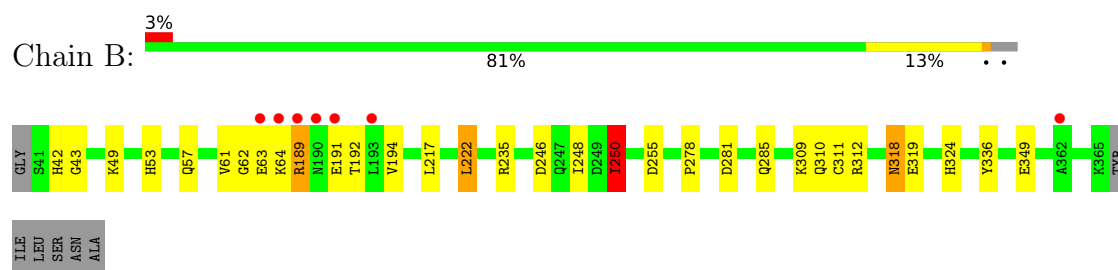
3 Residue-property plots [i](#)

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.

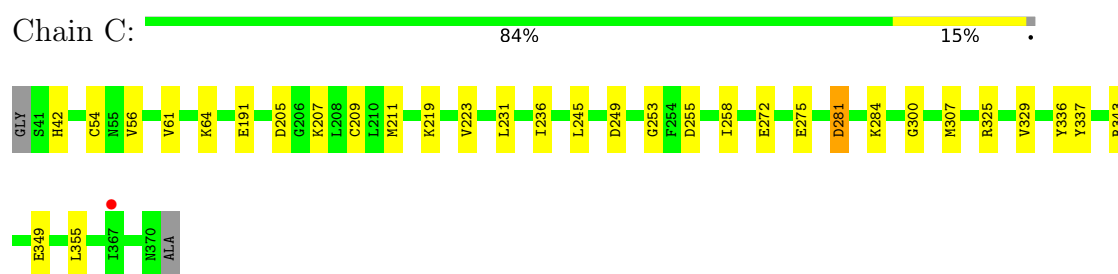
- Molecule 1: Inward rectifier potassium channel 2



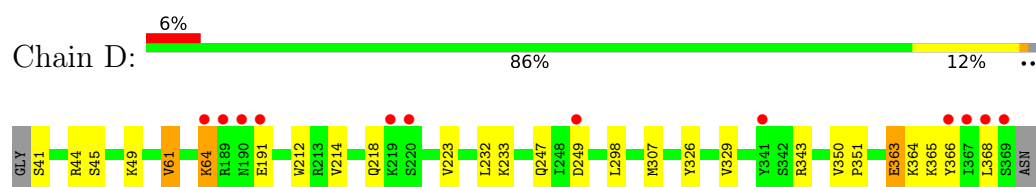
- Molecule 1: Inward rectifier potassium channel 2



- Molecule 1: Inward rectifier potassium channel 2



- Molecule 1: Inward rectifier potassium channel 2



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	140.67Å 98.88Å 98.09Å 90.00° 130.68° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.02 74.39 – 2.02	Depositor EDS
% Data completeness (in resolution range)	99.5 ((Not available)-2.02) 99.4 (74.39-2.02)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.177 , 0.229 0.181 , 0.235	Depositor DCC
R_{free} test set	3363 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	24.6	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.3	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	0.96	EDS
Total number of atoms	7303	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.19% 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: MPD, K

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	1.01	1/1689 (0.1%)	1.03	2/2285 (0.1%)
1	B	1.03	1/1646 (0.1%)	0.98	1/2226 (0.0%)
1	C	1.01	1/1689 (0.1%)	1.00	2/2285 (0.1%)
1	D	0.99	1/1685 (0.1%)	0.97	4/2278 (0.2%)
All	All	1.01	4/6709 (0.1%)	1.00	9/9074 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	223	VAL	CA-CB	5.99	1.62	1.54
1	B	250	ILE	CA-CB	5.80	1.61	1.54
1	C	236	ILE	CA-CB	5.70	1.61	1.54
1	A	42	HIS	N-CA	5.46	1.52	1.45

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	42	HIS	N-CA-C	7.17	120.35	109.23
1	A	204	ARG	NE-CZ-NH1	-5.59	115.91	121.50
1	C	300	GLY	N-CA-C	-5.50	103.38	110.69
1	D	351	PRO	CA-C-N	5.32	129.11	120.60
1	D	351	PRO	C-N-CA	5.32	129.11	120.60
1	C	42	HIS	N-CA-C	-5.12	101.41	109.50
1	B	191	GLU	N-CA-C	-5.10	107.03	113.20
1	D	350	VAL	CA-C-N	5.03	124.69	119.56
1	D	350	VAL	C-N-CA	5.03	124.69	119.56

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	1654	0	1619	22	0
1	B	1612	0	1577	25	0
1	C	1654	0	1619	20	0
1	D	1650	0	1624	14	0
2	A	1	0	0	0	0
3	A	8	0	14	0	0
3	B	8	0	14	0	0
3	C	8	0	14	0	0
3	D	8	0	14	1	0
4	A	192	0	0	3	0
4	B	169	0	0	7	0
4	C	164	0	0	8	0
4	D	175	0	0	5	0
All	All	7303	0	6495	78	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 6.

All (78) 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)
4:B:966:HOH:O	1:C:54:CYS:HB3	1.27	1.26
1:C:255:ASP:OD2	4:C:866:HOH:O	1.70	1.10
1:A:255:ASP:HB3	4:A:917:HOH:O	1.63	0.97
1:C:255:ASP:HB3	4:C:964:HOH:O	1.72	0.89
1:B:49:LYS:HE2	1:B:53:HIS:HD2	1.41	0.86
1:A:44:ARG:HH12	1:A:334:LYS:HG2	1.48	0.76
1:D:44:ARG:NH1	4:D:936:HOH:O	2.16	0.76
1:A:220:SER:HB2	4:A:979:HOH:O	1.86	0.74
1:B:49:LYS:CE	1:B:53:HIS:HD2	2.01	0.73
1:A:45:SER:OG	1:A:55:ASN:ND2	2.23	0.71
1:B:250:ILE:HD11	1:B:278:PRO:HG2	1.74	0.69
1:A:61:VAL:O	1:A:62:GLY:C	2.34	0.69
1:C:307:MET:HE1	4:C:965:HOH:O	1.93	0.69
4:C:874:HOH:O	1:D:307:MET:HE3	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:ASP:OD2	4:B:960:HOH:O	2.13	0.67
1:B:42:HIS:HD2	1:B:43:GLY:O	1.79	0.66
1:C:209:CYS:HB2	1:C:211:MET:HE2	1.79	0.65
1:A:281:ASP:OD2	1:A:359:ARG:NH1	2.29	0.64
1:C:56:VAL:O	1:C:219:LYS:NZ	2.27	0.63
1:A:44:ARG:NH1	1:A:334:LYS:HG2	2.14	0.63
1:B:49:LYS:CE	1:B:53:HIS:CD2	2.86	0.58
1:B:312:ARG:NH2	4:B:966:HOH:O	2.36	0.58
1:B:192:THR:HG22	4:B:964:HOH:O	2.04	0.57
1:A:41:SER:HA	1:D:233:LYS:HB2	1.86	0.57
1:C:205:ASP:OD1	4:C:946:HOH:O	2.17	0.57
1:B:250:ILE:CD1	1:B:278:PRO:HG2	2.35	0.56
1:B:222:LEU:HD11	1:B:309:LYS:HB2	1.87	0.56
1:B:217:LEU:HD11	1:B:311:CYS:SG	2.46	0.55
1:A:242:TYR:CE2	1:A:244:PRO:HG3	2.44	0.53
1:C:207:LYS:HD3	1:C:272:GLU:OE1	2.09	0.53
1:D:61:VAL:HG13	4:D:918:HOH:O	2.09	0.52
1:C:325:ARG:HD3	4:C:840:HOH:O	2.10	0.52
1:B:324:HIS:CD2	1:B:349:GLU:OE1	2.63	0.52
1:C:281:ASP:HB2	4:C:941:HOH:O	2.11	0.51
1:D:232:LEU:HD22	1:D:247:GLN:HG2	1.91	0.51
1:A:42:HIS:HD2	1:A:43:GLY:O	1.93	0.51
1:C:191:GLU:HG2	4:C:968:HOH:O	2.11	0.49
1:B:61:VAL:HG12	4:B:870:HOH:O	2.12	0.49
1:D:214:VAL:HG21	1:D:298:LEU:HD22	1.95	0.48
1:B:62:GLY:C	1:B:64:LYS:H	2.21	0.48
1:C:284:LYS:HD3	1:C:355:LEU:HD22	1.96	0.48
1:C:207:LYS:HD3	1:C:272:GLU:CD	2.40	0.47
1:B:248:ILE:HG12	4:B:919:HOH:O	2.14	0.47
1:D:249:ASP:HB3	4:D:881:HOH:O	2.15	0.47
1:B:49:LYS:HE2	1:B:53:HIS:CD2	2.33	0.46
1:B:318:ASN:C	1:B:318:ASN:HD22	2.23	0.46
1:A:284:LYS:HE3	1:A:288:ASP:OD2	2.15	0.46
1:C:253:GLY:HA3	1:C:258:ILE:HG13	1.97	0.46
1:A:318:ASN:HD22	1:A:318:ASN:C	2.24	0.45
1:D:191:GLU:O	1:D:218:GLN:HG2	2.16	0.45
1:A:232:LEU:HD11	1:A:295:VAL:CG2	2.47	0.45
1:A:318:ASN:ND2	1:A:319:GLU:HG3	2.32	0.45
1:D:329:VAL:HG12	1:D:343:ARG:HB2	1.98	0.44
1:A:329:VAL:HG12	1:A:343:ARG:HB2	1.99	0.44
1:C:329:VAL:HG12	1:C:343:ARG:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:TYR:HD1	1:C:337:TYR:O	2.01	0.44
1:B:217:LEU:HA	4:B:963:HOH:O	2.18	0.44
1:C:245:LEU:HD13	3:D:801:MPD:H11	1.99	0.44
1:A:232:LEU:HD11	1:A:295:VAL:HG21	2.00	0.44
1:D:363:GLU:C	1:D:365:LYS:H	2.25	0.43
1:B:64:LYS:O	1:B:189:ARG:C	2.62	0.43
1:A:62:GLY:O	1:A:63:GLU:CB	2.67	0.43
1:B:235:ARG:HD3	1:B:246:ASP:OD2	2.18	0.43
1:D:363:GLU:C	1:D:365:LYS:N	2.76	0.42
1:D:218:GLN:NE2	4:D:952:HOH:O	2.51	0.42
1:A:221:HIS:HE1	4:A:810:HOH:O	2.03	0.42
1:B:318:ASN:HD22	1:B:319:GLU:HG3	1.83	0.42
1:A:369:SER:OG	1:A:370:ASN:ND2	2.52	0.42
1:B:310:GLN:HB2	1:C:223:VAL:HG22	2.02	0.42
1:A:293:GLU:OE2	1:B:42:HIS:HE1	2.04	0.41
1:C:54:CYS:SG	1:C:219:LYS:HE3	2.61	0.41
1:A:220:SER:OG	1:A:303:GLU:HB3	2.20	0.41
1:B:57:GLN:HE21	1:B:336:TYR:HE1	1.69	0.41
1:D:45:SER:HB2	4:D:853:HOH:O	2.20	0.41
1:C:275:GLU:H	1:C:275:GLU:CD	2.28	0.41
1:D:212:TRP:HA	1:D:326:TYR:OH	2.20	0.41
1:B:318:ASN:ND2	1:B:319:GLU:HG3	2.35	0.40
1:A:196:SER:HB3	1:A:213:ARG:HB3	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	204/208 (98%)	196 (96%)	5 (2%)	3 (2%)	8	3
1	B	199/208 (96%)	188 (94%)	10 (5%)	1 (0%)	24	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	204/208 (98%)	201 (98%)	2 (1%)	1 (0%)	24	17
1	D	203/208 (98%)	197 (97%)	4 (2%)	2 (1%)	12	5
All	All	810/832 (97%)	782 (96%)	21 (3%)	7 (1%)	14	7

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	GLU
1	A	62	GLY
1	C	64	LYS
1	A	64	LYS
1	B	189	ARG
1	D	364	LYS
1	D	64	LYS

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	182/186 (98%)	177 (97%)	5 (3%)	39	37
1	B	177/186 (95%)	170 (96%)	7 (4%)	28	22
1	C	182/186 (98%)	177 (97%)	5 (3%)	39	37
1	D	182/186 (98%)	175 (96%)	7 (4%)	29	23
All	All	723/744 (97%)	699 (97%)	24 (3%)	33	29

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	191	GLU
1	A	220	SER
1	A	285	GLN
1	A	318	ASN
1	A	338	LYS

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Mol	Chain	Res	Type
1	B	63	GLU
1	B	194	VAL
1	B	222	LEU
1	B	250	ILE
1	B	281	ASP
1	B	285	GLN
1	B	318	ASN
1	C	61	VAL
1	C	231	LEU
1	C	249	ASP
1	C	281	ASP
1	C	349	GLU
1	D	41	SER
1	D	49	LYS
1	D	61	VAL
1	D	64	LYS
1	D	363	GLU
1	D	366	TYR
1	D	368	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	HIS
1	A	53	HIS
1	A	55	ASN
1	A	197	HIS
1	A	221	HIS
1	A	247	GLN
1	A	318	ASN
1	A	370	ASN
1	B	42	HIS
1	B	53	HIS
1	B	57	GLN
1	B	230	GLN
1	B	247	GLN
1	B	285	GLN
1	B	318	ASN
1	C	53	HIS
1	C	57	GLN
1	C	230	GLN
1	D	247	GLN

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Mol	Chain	Res	Type
1	D	335	HIS

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 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	MPD	B	802	-	7,7,7	0.53	0	9,10,10	0.63	0
3	MPD	D	801	-	7,7,7	0.58	0	9,10,10	0.97	1 (11%)
3	MPD	A	803	-	7,7,7	0.45	0	9,10,10	0.59	0
3	MPD	C	804	-	7,7,7	0.51	0	9,10,10	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	MPD	B	802	-	-	2/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MPD	D	801	-	-	0/5/5/5	-
3	MPD	A	803	-	-	1/5/5/5	-
3	MPD	C	804	-	-	2/5/5/5	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	801	MPD	O2-C2-CM	-2.15	101.27	107.99

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	803	MPD	O2-C2-C3-C4
3	B	802	MPD	O2-C2-C3-C4
3	C	804	MPD	O2-C2-C3-C4
3	B	802	MPD	CM-C2-C3-C4
3	C	804	MPD	CM-C2-C3-C4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	801	MPD	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	206/208 (99%)	-0.09	6 (2%) 53 53	14, 24, 51, 64	0
1	B	201/208 (96%)	-0.07	7 (3%) 47 46	12, 24, 48, 71	0
1	C	206/208 (99%)	-0.24	1 (0%) 87 87	15, 24, 47, 66	0
1	D	205/208 (98%)	-0.08	12 (5%) 28 27	14, 24, 50, 77	0
All	All	818/832 (98%)	-0.12	26 (3%) 50 49	12, 24, 51, 77	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	41	SER	4.7
1	B	193	LEU	4.1
1	B	190	ASN	3.8
1	D	367	ILE	3.5
1	A	62	GLY	3.4
1	B	189	ARG	3.3
1	B	64	LYS	3.3
1	B	362	ALA	3.2
1	D	368	LEU	3.2
1	D	191	GLU	3.1
1	A	190	ASN	2.7
1	D	369	SER	2.6
1	D	190	ASN	2.6
1	A	368	LEU	2.6
1	A	189	ARG	2.5
1	B	191	GLU	2.5
1	D	64	LYS	2.5
1	D	366	TYR	2.3
1	A	61	VAL	2.2
1	D	341	TYR	2.2
1	D	220	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	367	ILE	2.1
1	D	249	ASP	2.0
1	B	63	GLU	2.0
1	D	189	ARG	2.0
1	D	219	LYS	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($\text{\AA}^2$)	Q<0.9
3	MPD	A	803	8/8	0.92	0.10	32,36,37,38	0
3	MPD	B	802	8/8	0.92	0.09	24,27,27,28	0
3	MPD	C	804	8/8	0.92	0.09	30,33,34,35	0
3	MPD	D	801	8/8	0.92	0.09	22,23,25,26	0
2	K	A	800	1/1	0.96	0.06	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.