



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:49 AM GMT

PDB ID : 3Q4U  
Title : Crystal structure of the ACVR1 kinase domain in complex with LDN-193189  
Authors : Chaikuad, A.; Sanvitale, C.; Cooper, C.D.O.; Mahajan, P.; Daga, N.; Petrie, K.; Alfano, I.; Gileadi, O.; Fedorov, O.; Allerston, C.K.; Krojer, T.; Vollmar, M.; von Delft, F.; Weigelt, J.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Bullock, A.; Structural Genomics Consortium (SGC)  
Deposited on : 2010-12-24  
Resolution : 1.82 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](mailto: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.

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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

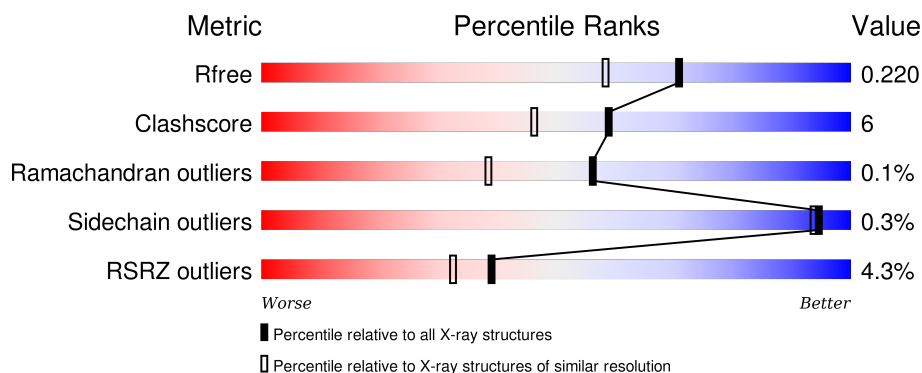
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.82 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	5422 (1.84-1.80)
Clashscore	102246	6347 (1.84-1.80)
Ramachandran outliers	100387	6276 (1.84-1.80)
Sidechain outliers	100360	6276 (1.84-1.80)
RSRZ outliers	91569	5439 (1.84-1.80)

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  $\geq 3$ , 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	301	<div> <div>2%</div> <div>88%</div> <div>10%</div> <div>.</div> </div>
1	B	301	<div> <div>8%</div> <div>90%</div> <div>10%</div> </div>
1	C	301	<div> <div>4%</div> <div>90%</div> <div>7%</div> <div>..</div> </div>
1	D	301	<div> <div>3%</div> <div>86%</div> <div>14%</div> <div>.</div> </div>

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
3	EDO	A	1	-	-	-	X
3	EDO	A	500	-	-	-	X
3	EDO	B	8	-	-	-	X
3	EDO	C	10	-	-	-	X
3	EDO	C	9[A]	-	-	-	X
3	EDO	C	9[B]	-	-	-	X
3	EDO	D	14[A]	-	-	-	X
3	EDO	D	14[B]	-	-	-	X
4	FLC	A	501	-	-	-	X
4	FLC	A	502	-	-	-	X
4	FLC	B	5	-	-	-	X
4	FLC	B	500	-	-	-	X
4	FLC	B	501	-	-	-	X
4	FLC	B	6	-	-	-	X
4	FLC	C	12	-	-	-	X
4	FLC	C	3	-	-	-	X
4	FLC	D	10	-	-	-	X
4	FLC	D	11	-	-	-	X
4	FLC	D	9	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11134 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.

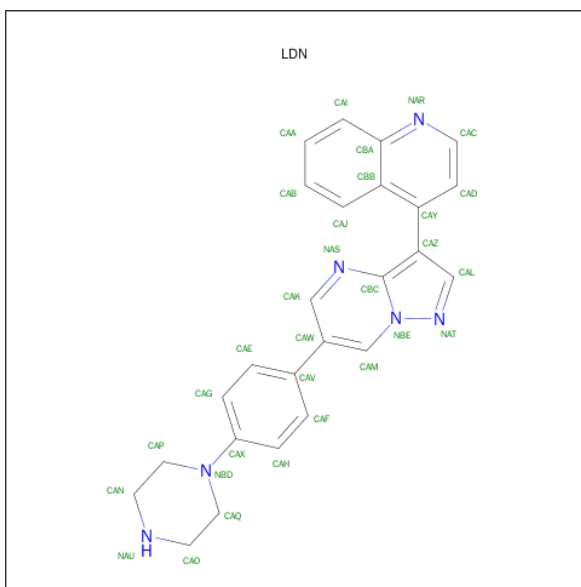
- Molecule 1 is a protein called Activin receptor type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	0	10	0
			2435	1550	421	446	18			
1	B	300	Total	C	N	O	S	0	6	0
			2408	1533	420	438	17			
1	C	296	Total	C	N	O	S	0	17	0
			2459	1570	421	451	17			
1	D	299	Total	C	N	O	S	0	12	0
			2465	1568	426	454	17			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	199	SER	-	EXPRESSION TAG	UNP Q04771
A	200	MET	-	EXPRESSION TAG	UNP Q04771
A	207	ASP	GLN	ENGINEERED MUTATION	UNP Q04771
B	199	SER	-	EXPRESSION TAG	UNP Q04771
B	200	MET	-	EXPRESSION TAG	UNP Q04771
B	207	ASP	GLN	ENGINEERED MUTATION	UNP Q04771
C	199	SER	-	EXPRESSION TAG	UNP Q04771
C	200	MET	-	EXPRESSION TAG	UNP Q04771
C	207	ASP	GLN	ENGINEERED MUTATION	UNP Q04771
D	199	SER	-	EXPRESSION TAG	UNP Q04771
D	200	MET	-	EXPRESSION TAG	UNP Q04771
D	207	ASP	GLN	ENGINEERED MUTATION	UNP Q04771

- Molecule 2 is 4-[6-(4-PIPERAZIN-1-YLPHENYL)PYRAZOLO[1,5-A]PYRIMIDIN-3-YL]QUINOLINE (three-letter code: LDN) (formula: C<sub>25</sub>H<sub>22</sub>N<sub>6</sub>).



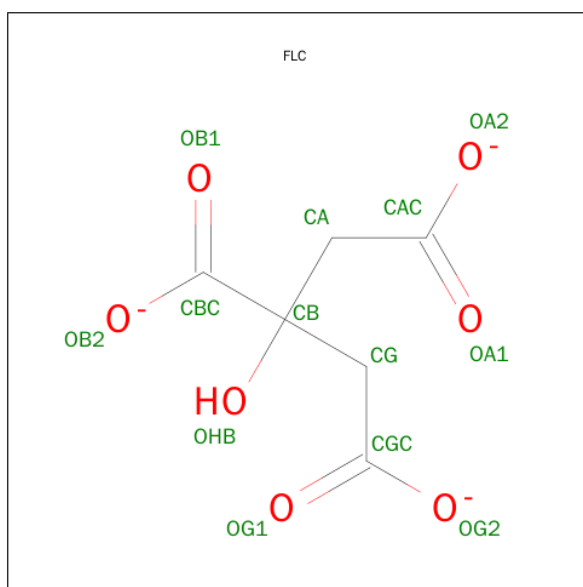
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			31	25	6		
2	B	1	Total	C	N	0	0
			31	25	6		
2	C	1	Total	C	N	0	0
			31	25	6		
2	D	1	Total	C	N	0	0
			31	25	6		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 8 4 4	0	1
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 8 4 4	0	1
3	D	1	Total C O 8 4 4	0	1

- Molecule 4 is CITRATE ANION (three-letter code: FLC) (formula:  $C_6H_5O_7$ ).



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

- Molecule 5 is water.

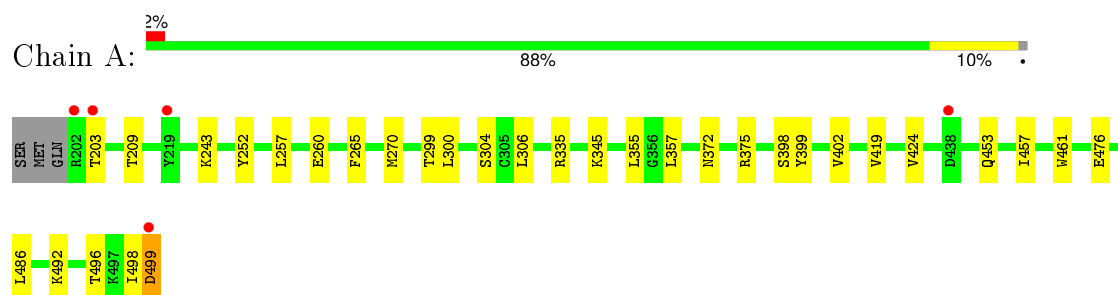
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	254	Total 254	O 254	0	0
5	B	218	Total 218	O 218	0	0
5	C	254	Total 254	O 254	0	0
5	D	293	Total 293	O 293	0	0



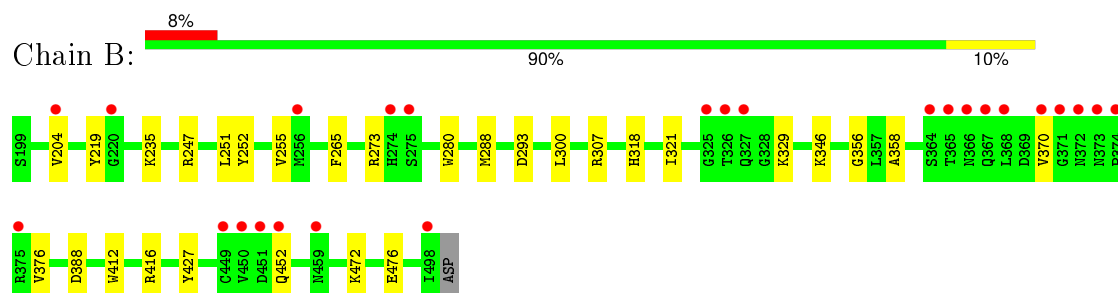
### 3 Residue-property plots [i](#)

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.

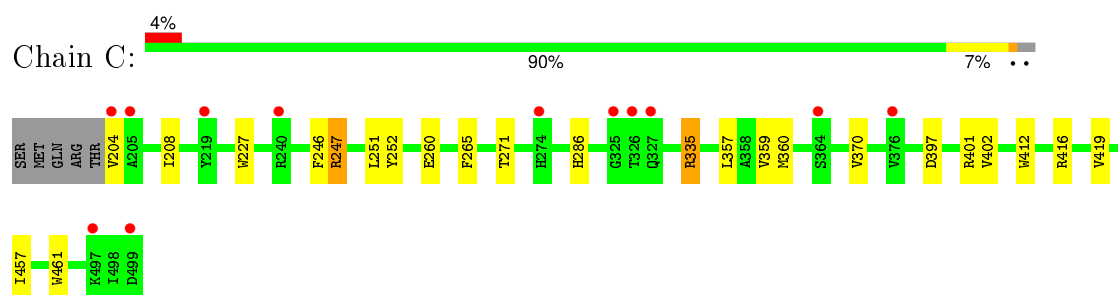
#### • Molecule 1: Activin receptor type-1



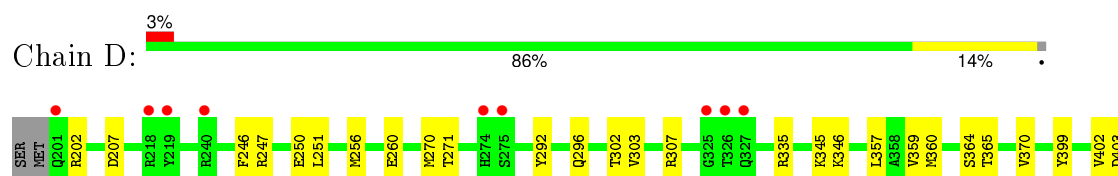
#### • Molecule 1: Activin receptor type-1



#### • Molecule 1: Activin receptor type-1



#### • Molecule 1: Activin receptor type-1



R417	Y418	Y419	Y424	R428	Y434	Y435	D438	R446	Y447	Y448	Q452	I457	W461	W474	D499
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.60Å 98.70Å 83.85Å 90.00° 117.42° 90.00°	Depositor
Resolution (Å)	37.22 – 1.82 37.21 – 1.82	Depositor EDS
% Data completeness (in resolution range)	99.1 (37.22-1.82) 99.1 (37.21-1.82)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.80 (at 1.82Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, $R_{free}$	0.163 , 0.219 0.166 , 0.220	Depositor DCC
$R_{free}$ test set	5385 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.9	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 44.1	EDS
Estimated twinning fraction	0.006 for -h-l,k,h 0.006 for l,k,-h-l 0.018 for h,-k,-h-l 0.020 for -h-l,-k,l 0.018 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 107170 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	11134	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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: FLC, EDO, LDN

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	0.73	0/2519	0.69	0/3414
1	B	0.66	0/2480	0.67	0/3365
1	C	0.78	0/2565	0.75	3/3478 (0.1%)
1	D	0.79	0/2553	0.76	4/3460 (0.1%)
All	All	0.74	0/10117	0.72	7/13717 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	417	ARG	NE-CZ-NH1	7.03	123.82	120.30
1	C	247	ARG	NE-CZ-NH2	-6.75	116.93	120.30
1	C	335	ARG	NE-CZ-NH2	6.36	123.48	120.30
1	D	247	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	D	403	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	D	417	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	C	247	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	2435	0	2449	23	0
1	B	2408	0	2399	26	0
1	C	2459	0	2482	25	0
1	D	2465	0	2471	30	0
2	A	31	0	22	0	0
2	B	31	0	22	2	0
2	C	31	0	22	1	0
2	D	31	0	22	0	0
3	A	20	0	30	4	0
3	B	8	0	12	2	0
3	C	16	0	24	5	0
3	D	24	0	36	2	0
4	A	26	0	10	3	0
4	B	52	0	20	5	0
4	C	39	0	15	4	0
4	D	39	0	15	5	0
5	A	254	0	0	2	0
5	B	218	0	0	7	0
5	C	254	0	0	6	0
5	D	293	0	0	9	0
All	All	11134	0	10051	116	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 (116) 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:C:247:ARG:HD3	3:C:9[B]:EDO:H21	1.68	0.76
4:D:11:FLC:OG2	5:D:1152:HOH:O	2.09	0.70
4:D:9:FLC:OA2	4:D:9:FLC:CBC	2.37	0.69
1:C:397[B]:ASP:OD2	1:C:401[B]:ARG:CZ	2.40	0.69
1:B:293:ASP:OD2	5:B:972:HOH:O	2.11	0.66
1:C:397[B]:ASP:OD2	1:C:401[B]:ARG:NH2	2.29	0.65
1:A:492:LYS:O	1:A:496[B]:THR:HG23	1.98	0.64
4:C:3:FLC:HA1	4:C:3:FLC:OG2	1.97	0.64
1:A:498:ILE:O	5:A:552:HOH:O	2.16	0.63
1:C:286:HIS:CE1	4:C:3:FLC:HG2	2.33	0.62
1:D:271[B]:THR:HG23	5:D:650:HOH:O	2.00	0.62
1:D:302[B]:THR:HG22	1:D:418:MET:CE	2.30	0.62
1:C:260:GLU:HG3	5:C:568:HOH:O	2.00	0.61
4:A:501:FLC:CBC	4:A:501:FLC:OA2	2.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:345:LYS:NZ	4:D:10:FLC:HA1	2.17	0.60
1:D:251:LEU:HD21	1:D:360[B]:MET:SD	2.41	0.60
4:C:3:FLC:OB2	4:C:3:FLC:OA2	2.21	0.58
1:D:303:VAL:HG21	5:D:672:HOH:O	2.03	0.58
4:B:501:FLC:HG1	5:B:984:HOH:O	2.04	0.57
1:B:247:ARG:HD3	1:B:358:ALA:O	2.04	0.57
1:A:243:LYS:HD3	1:A:372:ASN:O	2.05	0.57
1:D:335:ARG:HD3	1:D:357:LEU:O	2.06	0.56
1:C:260:GLU:CG	5:C:568:HOH:O	2.52	0.55
1:C:335:ARG:HD3	1:C:357:LEU:O	2.06	0.55
1:B:376:VAL:HG11	5:B:776:HOH:O	2.06	0.55
1:B:412:TRP:CZ2	1:B:416:ARG:HD2	2.40	0.55
1:A:304:SER:OG	3:A:500:EDO:H22	2.07	0.55
4:C:500:FLC:HG1	5:C:624:HOH:O	2.07	0.55
1:A:306:LEU:HD13	1:A:499:ASP:HB3	1.89	0.54
1:C:370[B]:VAL:HG22	5:C:559:HOH:O	2.08	0.54
1:A:476:GLU:HB3	1:A:486:LEU:HG	1.88	0.54
1:A:299:THR:O	3:A:4:EDO:H22	2.08	0.54
1:C:359:VAL:HG22	1:C:370[B]:VAL:HA	1.90	0.54
1:A:419:VAL:HG22	1:A:424:VAL:HG13	1.90	0.53
1:A:345:LYS:NZ	4:A:502:FLC:OHB	2.42	0.53
1:B:300:LEU:HA	3:B:8:EDO:C1	2.39	0.53
1:D:370:VAL:HG12	1:D:370:VAL:O	2.09	0.52
3:D:13[B]:EDO:C2	5:D:1064:HOH:O	2.57	0.52
1:C:359:VAL:HG22	1:C:370[A]:VAL:HA	1.91	0.52
1:D:438:ASP:HA	3:D:13[B]:EDO:H11	1.92	0.51
1:C:401[B]:ARG:NH1	5:C:1041:HOH:O	2.35	0.51
1:C:402:VAL:HG13	5:C:1025:HOH:O	2.10	0.51
4:B:6:FLC:OB2	4:B:6:FLC:CGC	2.59	0.51
1:B:251:LEU:O	1:B:255:VAL:HB	2.12	0.50
1:B:346:LYS:HB2	4:B:5:FLC:OB1	2.11	0.50
1:A:399:TYR:O	1:A:402[B]:VAL:HG22	2.12	0.49
1:C:251:LEU:HD21	1:C:360[B]:MET:SD	2.52	0.49
4:B:500:FLC:OG2	4:B:500:FLC:OHB	2.30	0.49
1:B:300:LEU:HA	3:B:8:EDO:H12	1.95	0.49
1:D:307:ARG:NH1	5:D:726:HOH:O	2.44	0.48
1:D:202:ARG:HA	1:D:207:ASP:OD1	2.13	0.48
1:A:357:LEU:HD21	1:A:375:ARG:HB3	1.96	0.48
1:A:300:LEU:HA	3:A:500:EDO:C2	2.43	0.48
1:D:399:TYR:O	1:D:402:VAL:HG22	2.14	0.47
1:C:412:TRP:CZ2	1:C:416:ARG:HD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:256:MET:HB2	5:D:1055:HOH:O	2.13	0.47
1:C:246:PHE:HD2	3:C:9[B]:EDO:H22	1.79	0.47
1:B:307:ARG:NH1	5:B:674:HOH:O	2.48	0.47
1:B:288[B]:MET:HE1	5:B:630:HOH:O	2.13	0.47
1:A:402[A]:VAL:HG13	5:A:571:HOH:O	2.16	0.46
4:B:500:FLC:CBC	4:B:500:FLC:OA1	2.63	0.46
1:D:370:VAL:CG1	1:D:370:VAL:O	2.64	0.45
1:C:246:PHE:HD2	3:C:9[A]:EDO:H22	1.81	0.45
1:B:376:VAL:HG21	5:B:990:HOH:O	2.16	0.45
1:A:300:LEU:HA	3:A:500:EDO:H22	1.97	0.45
1:A:260:GLU:HA	4:A:502:FLC:HA1	1.98	0.45
1:B:252:TYR:CD1	1:B:265:PHE:HB2	2.51	0.45
1:B:472:LYS:O	1:B:476:GLU:HG3	2.16	0.45
1:D:345:LYS:HD3	4:D:10:FLC:OG2	2.17	0.45
1:D:335:ARG:CD	1:D:359:VAL:HG13	2.47	0.45
1:B:288[A]:MET:HB3	1:B:288[A]:MET:HE3	1.88	0.44
1:A:457:ILE:HG23	1:A:461:TRP:CE3	2.52	0.44
1:D:448:VAL:O	1:D:452:GLN:HA	2.18	0.44
1:D:335:ARG:HD2	1:D:359:VAL:HG13	2.00	0.44
1:B:318:HIS:O	1:B:329:LYS:HE3	2.18	0.44
1:C:457:ILE:HG23	1:C:461:TRP:CE3	2.53	0.44
1:D:428:LYS:NZ	5:D:1106:HOH:O	2.51	0.43
1:C:251:LEU:HD21	1:C:360[B]:MET:CE	2.47	0.43
2:B:1:LDN:CBC	2:B:1:LDN:HAJ	2.49	0.43
1:A:335:ARG:HD3	1:A:357:LEU:O	2.18	0.43
1:B:204:VAL:HG11	1:B:280:TRP:CE2	2.53	0.43
1:A:257:LEU:HD23	1:A:355:LEU:CD1	2.49	0.43
2:C:4:LDN:HAQ	2:C:4:LDN:HAG	1.80	0.43
1:B:219:TYR:HB2	1:B:235:LYS:NZ	2.33	0.43
1:C:271[B]:THR:HG23	3:C:11:EDO:H22	2.01	0.43
1:A:398:SER:O	1:A:402[B]:VAL:HG13	2.18	0.43
1:B:219:TYR:HD2	1:B:235:LYS:HZ1	1.62	0.43
1:B:247:ARG:HD2	1:B:356:GLY:O	2.19	0.42
1:D:246:PHE:CE2	1:D:250:GLU:HG3	2.54	0.42
1:D:303:VAL:HG21	5:D:607:HOH:O	2.19	0.42
1:C:252:TYR:CD1	1:C:265:PHE:HB2	2.54	0.42
1:D:434:VAL:HG23	1:D:435:VAL:HG13	2.02	0.42
1:A:203:THR:O	1:B:273:ARG:NH1	2.41	0.42
1:D:364:SER:OG	1:D:365:THR:HG23	2.19	0.42
1:B:427:TYR:C	1:B:427:TYR:CD2	2.92	0.42
1:A:209:THR:OG1	1:C:419:VAL:HG21	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:461:TRP:CZ3	1:D:474:MET:HE1	2.55	0.41
1:A:453[A]:GLN:HA	1:A:453[A]:GLN:OE1	2.20	0.41
1:B:288[B]:MET:HE2	1:B:288[B]:MET:HB3	1.98	0.41
1:D:457:ILE:HG23	1:D:461:TRP:CE3	2.55	0.41
1:C:335:ARG:HD2	1:C:359:VAL:CG2	2.50	0.41
1:C:204:VAL:O	1:C:208:ILE:HG13	2.21	0.41
1:C:247:ARG:HD3	3:C:9[A]:EDO:H21	2.02	0.41
1:A:252:TYR:CD1	1:A:265:PHE:HB2	2.56	0.41
1:D:251:LEU:CD2	1:D:360[B]:MET:SD	3.08	0.41
2:B:1:LDN:HAPA	2:B:1:LDN:HAH	1.80	0.41
1:B:452:GLN:HG2	5:B:771:HOH:O	2.21	0.41
1:D:260[A]:GLU:OE1	1:D:345:LYS:NZ	2.53	0.41
1:C:204:VAL:HG13	1:C:227:TRP:CE2	2.56	0.40
1:D:446:LYS:NZ	5:D:595:HOH:O	2.21	0.40
1:D:346:LYS:HD2	4:D:9:FLC:HG1	2.04	0.40
1:B:388:ASP:C	1:B:388:ASP:OD1	2.59	0.40
1:D:292:TYR:O	1:D:296:GLN:HG2	2.21	0.40
1:D:419:VAL:HG22	1:D:424:VAL:HB	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	306/301 (102%)	301 (98%)	5 (2%)	0	100	100
1	B	304/301 (101%)	293 (96%)	10 (3%)	1 (0%)	46	29
1	C	311/301 (103%)	306 (98%)	5 (2%)	0	100	100
1	D	309/301 (103%)	304 (98%)	5 (2%)	0	100	100
All	All	1230/1204 (102%)	1204 (98%)	25 (2%)	1 (0%)	56	38

All (1) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	B	370	VAL

### 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	275/270 (102%)	273 (99%)	2 (1%)	88	85
1	B	266/270 (98%)	266 (100%)	0	100	100
1	C	280/270 (104%)	280 (100%)	0	100	100
1	D	278/270 (103%)	277 (100%)	1 (0%)	93	92
All	All	1099/1080 (102%)	1096 (100%)	3 (0%)	94	93

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	270	MET
1	A	499	ASP
1	D	270	MET

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

### 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

33 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	EDO	A	1	-	3,3,3	0.51	0	2,2,2	0.33	0
3	EDO	A	2	-	3,3,3	0.19	0	2,2,2	0.36	0
2	LDN	A	3	-	31,36,36	1.18	2 (6%)	40,51,51	2.04	10 (25%)
3	EDO	A	4	-	3,3,3	0.53	0	2,2,2	0.61	0
3	EDO	A	5	-	3,3,3	0.62	0	2,2,2	0.61	0
3	EDO	A	500	-	3,3,3	0.47	0	2,2,2	0.54	0
4	FLC	A	501	-	3,12,12	0.49	0	3,17,17	1.66	1 (33%)
4	FLC	A	502	-	3,12,12	1.08	0	3,17,17	2.52	2 (66%)
2	LDN	B	1	-	31,36,36	1.19	3 (9%)	40,51,51	1.79	6 (15%)
4	FLC	B	5	-	3,12,12	3.14	1 (33%)	3,17,17	3.53	2 (66%)
4	FLC	B	500	-	3,12,12	0.93	0	3,17,17	3.57	2 (66%)
4	FLC	B	501	-	3,12,12	1.97	1 (33%)	3,17,17	8.63	3 (100%)
4	FLC	B	6	-	3,12,12	0.51	0	3,17,17	2.23	1 (33%)
3	EDO	B	7	-	3,3,3	0.56	0	2,2,2	0.59	0
3	EDO	B	8	-	3,3,3	0.63	0	2,2,2	0.23	0
3	EDO	C	10	-	3,3,3	0.49	0	2,2,2	0.66	0
3	EDO	C	11	-	3,3,3	0.44	0	2,2,2	1.05	0
4	FLC	C	12	-	3,12,12	1.75	1 (33%)	3,17,17	3.16	1 (33%)
4	FLC	C	3	-	3,12,12	3.16	1 (33%)	3,17,17	3.55	2 (66%)
2	LDN	C	4	-	31,36,36	1.04	2 (6%)	40,51,51	2.06	8 (20%)
4	FLC	C	500	-	3,12,12	1.68	0	3,17,17	1.12	0
3	EDO	C	9[A]	-	3,3,3	0.50	0	2,2,2	0.16	0
3	EDO	C	9[B]	-	3,3,3	0.44	0	2,2,2	0.21	0
4	FLC	D	10	-	3,12,12	2.26	1 (33%)	3,17,17	7.24	3 (100%)
4	FLC	D	11	-	3,12,12	0.39	0	3,17,17	2.25	2 (66%)
3	EDO	D	12	-	3,3,3	0.48	0	2,2,2	0.38	0
3	EDO	D	13[A]	-	3,3,3	0.56	0	2,2,2	0.30	0
3	EDO	D	13[B]	-	3,3,3	0.37	0	2,2,2	0.58	0
3	EDO	D	14[A]	-	3,3,3	0.56	0	2,2,2	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	D	14[B]	-	3,3,3	0.62	0	2,2,2	0.23	0
2	LDN	D	2	-	31,36,36	1.22	4 (12%)	40,51,51	1.90	9 (22%)
3	EDO	D	6	-	3,3,3	0.72	0	2,2,2	0.43	0
4	FLC	D	9	-	3,12,12	1.10	0	3,17,17	3.85	2 (66%)

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	EDO	A	1	-	-	0/1/1/1	0/0/0/0
3	EDO	A	2	-	-	0/1/1/1	0/0/0/0
2	LDN	A	3	-	-	0/11/20/20	0/6/6/6
3	EDO	A	4	-	-	0/1/1/1	0/0/0/0
3	EDO	A	5	-	-	0/1/1/1	0/0/0/0
3	EDO	A	500	-	-	0/1/1/1	0/0/0/0
4	FLC	A	501	-	-	0/6/16/16	0/0/0/0
4	FLC	A	502	-	-	0/6/16/16	0/0/0/0
2	LDN	B	1	-	-	0/11/20/20	0/6/6/6
4	FLC	B	5	-	-	0/6/16/16	0/0/0/0
4	FLC	B	500	-	-	0/6/16/16	0/0/0/0
4	FLC	B	501	-	-	0/6/16/16	0/0/0/0
4	FLC	B	6	-	-	0/6/16/16	0/0/0/0
3	EDO	B	7	-	-	0/1/1/1	0/0/0/0
3	EDO	B	8	-	-	0/1/1/1	0/0/0/0
3	EDO	C	10	-	-	0/1/1/1	0/0/0/0
3	EDO	C	11	-	-	0/1/1/1	0/0/0/0
4	FLC	C	12	-	-	0/6/16/16	0/0/0/0
4	FLC	C	3	-	-	0/6/16/16	0/0/0/0
2	LDN	C	4	-	-	0/11/20/20	0/6/6/6
4	FLC	C	500	-	-	0/6/16/16	0/0/0/0
3	EDO	C	9[A]	-	-	0/1/1/1	0/0/0/0
3	EDO	C	9[B]	-	-	0/1/1/1	0/0/0/0
4	FLC	D	10	-	-	0/6/16/16	0/0/0/0
4	FLC	D	11	-	-	0/6/16/16	0/0/0/0
3	EDO	D	12	-	-	0/1/1/1	0/0/0/0
3	EDO	D	13[A]	-	-	0/1/1/1	0/0/0/0
3	EDO	D	13[B]	-	-	0/1/1/1	0/0/0/0
3	EDO	D	14[A]	-	-	0/1/1/1	0/0/0/0
3	EDO	D	14[B]	-	-	0/1/1/1	0/0/0/0
2	LDN	D	2	-	-	0/11/20/20	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	D	6	-	-	0/1/1/1	0/0/0/0
4	FLC	D	9	-	-	0/6/16/16	0/0/0/0

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	LDN	CAV-CAW	-3.14	1.40	1.49
2	B	1	LDN	CAV-CAW	-3.07	1.41	1.49
2	A	3	LDN	CAV-CAW	-2.93	1.41	1.49
4	C	12	FLC	CG-CB	-2.79	1.50	1.54
2	C	4	LDN	CAZ-CAY	-2.66	1.43	1.49
2	B	1	LDN	CAZ-CAY	-2.36	1.43	1.49
2	B	1	LDN	CBA-NAR	-2.20	1.33	1.37
2	D	2	LDN	CAZ-CAY	-2.05	1.44	1.49
2	C	4	LDN	CAH-CAF	2.12	1.42	1.38
2	D	2	LDN	CAB-CAJ	2.15	1.41	1.36
2	D	2	LDN	CAK-NAS	2.30	1.35	1.31
4	B	501	FLC	OHB-CB	3.03	1.48	1.43
4	D	10	FLC	CG-CB	3.10	1.59	1.54
2	A	3	LDN	CAK-NAS	3.30	1.37	1.31
4	B	5	FLC	OHB-CB	5.39	1.51	1.43
4	C	3	FLC	OHB-CB	5.44	1.52	1.43

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	501	FLC	CB-CA-CAC	-13.43	93.49	114.96
4	D	10	FLC	CB-CG-CGC	-9.42	99.90	114.96
4	B	500	FLC	CB-CG-CGC	-5.51	106.14	114.96
4	D	9	FLC	CB-CA-CAC	-5.28	106.52	114.96
4	C	12	FLC	CB-CA-CAC	-5.12	106.77	114.96
2	C	4	LDN	CAW-CAK-NAS	-4.15	120.21	125.46
4	D	9	FLC	CB-CG-CGC	-3.78	108.91	114.96
4	B	6	FLC	CB-CA-CAC	-3.52	109.34	114.96
2	B	1	LDN	CAW-CAK-NAS	-3.36	121.21	125.46
2	A	3	LDN	CAG-CAX-NBD	-3.08	117.24	121.38
2	D	2	LDN	CAW-CAK-NAS	-2.90	121.79	125.46
2	D	2	LDN	CBB-CBA-NAR	-2.87	119.82	122.88
4	A	502	FLC	CB-CG-CGC	-2.82	110.44	114.96
4	A	501	FLC	CB-CA-CAC	-2.70	110.63	114.96
4	B	500	FLC	CB-CA-CAC	-2.68	110.67	114.96
4	B	501	FLC	CB-CG-CGC	-2.68	110.67	114.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	11	FLC	CB-CA-CAC	-2.68	110.68	114.96
2	A	3	LDN	CAW-CAK-NAS	-2.59	122.18	125.46
2	A	3	LDN	CAD-CAC-NAR	-2.56	120.52	124.56
2	D	2	LDN	CAH-CAX-NBD	-2.39	118.18	121.38
2	C	4	LDN	CAN-CAP-NBD	-2.28	105.10	110.70
2	C	4	LDN	CBB-CBA-NAR	-2.24	120.49	122.88
2	D	2	LDN	CAQ-NBD-CAX	2.15	123.67	117.92
2	A	3	LDN	CAC-CAD-CAY	2.18	121.69	119.98
2	A	3	LDN	CAC-NAR-CBA	2.33	120.82	116.87
2	B	1	LDN	CAK-NAS-CBC	2.35	119.97	116.86
4	B	5	FLC	CG-CB-CA	2.51	115.80	109.81
4	D	11	FLC	CG-CB-CA	2.72	116.32	109.81
2	A	3	LDN	CAQ-NBD-CAP	2.76	117.38	111.59
2	D	2	LDN	CAK-NAS-CBC	2.80	120.57	116.86
2	A	3	LDN	CAZ-CAY-CBB	2.92	125.61	121.44
2	C	4	LDN	CAM-CAW-CAK	2.93	118.74	115.45
2	B	1	LDN	CAM-CAW-CAK	3.00	118.81	115.45
2	D	2	LDN	CAQ-NBD-CAP	3.02	117.92	111.59
2	D	2	LDN	CAC-NAR-CBA	3.03	122.01	116.87
2	C	4	LDN	CAK-NAS-CBC	3.08	120.93	116.86
2	C	4	LDN	CAZ-CAY-CBB	3.08	125.83	121.44
2	A	3	LDN	CAM-CAW-CAK	3.22	119.06	115.45
2	B	1	LDN	CAQ-NBD-CAP	3.22	118.36	111.59
4	A	502	FLC	CG-CB-CA	3.32	117.75	109.81
4	C	3	FLC	CB-CG-CGC	3.46	120.49	114.96
2	D	2	LDN	CAY-CBB-CBA	3.58	119.33	117.46
2	B	1	LDN	CAY-CBB-CBA	4.07	119.58	117.46
4	D	10	FLC	CG-CB-CA	4.60	120.81	109.81
2	C	4	LDN	CAY-CBB-CBA	4.82	119.98	117.46
2	A	3	LDN	CAY-CBB-CBA	4.88	120.01	117.46
4	C	3	FLC	CG-CB-CA	4.98	121.72	109.81
4	B	5	FLC	CB-CG-CGC	5.41	123.60	114.96
4	B	501	FLC	CG-CB-CA	6.01	124.18	109.81
2	B	1	LDN	CAL-NAT-NBE	6.72	108.76	103.70
4	D	10	FLC	CB-CA-CAC	6.88	125.95	114.96
2	A	3	LDN	CAL-NAT-NBE	7.11	109.05	103.70
2	D	2	LDN	CAL-NAT-NBE	7.18	109.10	103.70
2	C	4	LDN	CAL-NAT-NBE	7.48	109.33	103.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

20 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4	EDO	1	0
3	A	500	EDO	3	0
4	A	501	FLC	1	0
4	A	502	FLC	2	0
2	B	1	LDN	2	0
4	B	5	FLC	1	0
4	B	500	FLC	2	0
4	B	501	FLC	1	0
4	B	6	FLC	1	0
3	B	8	EDO	2	0
3	C	11	EDO	1	0
4	C	3	FLC	3	0
2	C	4	LDN	1	0
4	C	500	FLC	1	0
3	C	9[A]	EDO	2	0
3	C	9[B]	EDO	2	0
4	D	10	FLC	2	0
4	D	11	FLC	1	0
3	D	13[B]	EDO	2	0
4	D	9	FLC	2	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	298/301 (99%)	-0.31	5 (1%) 73 69	13, 24, 47, 69	0
1	B	300/301 (99%)	0.18	25 (8%) 14 11	14, 32, 71, 108	0
1	C	296/301 (98%)	-0.19	12 (4%) 41 35	10, 22, 47, 69	0
1	D	299/301 (99%)	-0.17	9 (3%) 54 48	10, 21, 49, 94	0
All	All	1193/1204 (99%)	-0.12	51 (4%) 39 32	10, 24, 56, 108	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	372	ASN	7.6
1	D	201	GLN	7.4
1	B	371	GLY	5.9
1	B	450	VAL	5.8
1	B	375	ARG	5.6
1	D	326	THR	5.4
1	B	370	VAL	5.3
1	B	374	PRO	5.1
1	B	366	ASN	4.9
1	C	204	VAL	4.6
1	D	275	SER	4.5
1	B	256	MET	4.4
1	D	274	HIS	4.2
1	D	325	GLY	4.1
1	D	219[A]	TYR	4.0
1	B	326	THR	3.9
1	B	373	ASN	3.8
1	C	326	THR	3.8
1	B	274	HIS	3.4
1	B	327	GLN	3.4
1	B	498	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	202	ARG	3.3
1	B	368	LEU	3.3
1	C	219[A]	TYR	3.1
1	C	376	VAL	3.1
1	B	364	SER	3.1
1	C	325	GLY	3.1
1	A	219	TYR	3.0
1	B	325	GLY	3.0
1	C	499	ASP	3.0
1	D	327	GLN	2.9
1	B	449	CYS	2.7
1	A	499	ASP	2.7
1	B	459	ASN	2.6
1	C	240	ARG	2.6
1	C	327	GLN	2.6
1	D	240	ARG	2.5
1	B	275	SER	2.5
1	B	365	THR	2.4
1	D	218	ARG	2.4
1	A	203	THR	2.3
1	B	451	ASP	2.2
1	B	367	GLN	2.2
1	B	452	GLN	2.2
1	C	205	ALA	2.1
1	C	497	LYS	2.0
1	C	364	SER	2.0
1	B	220	GLY	2.0
1	A	438	ASP	2.0
1	B	204	VAL	2.0
1	C	274	HIS	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	FLC	B	6	13/13	0.85	0.29	9.59	36,44,51,53	0
3	EDO	D	14[A]	4/4	0.78	0.23	8.94	27,44,44,46	4
4	FLC	B	500	13/13	0.86	0.19	7.32	29,42,45,49	0
4	FLC	D	11	13/13	0.86	0.23	6.75	23,47,52,53	0
4	FLC	D	9	13/13	0.90	0.25	6.47	28,39,47,62	0
3	EDO	A	500	4/4	0.92	0.14	6.37	29,31,42,44	0
3	EDO	D	14[B]	4/4	0.78	0.23	5.95	36,45,47,49	4
4	FLC	D	10	13/13	0.80	0.27	5.59	19,44,53,62	0
4	FLC	B	5	13/13	0.89	0.23	5.40	26,34,49,50	0
4	FLC	C	3	13/13	0.72	0.27	5.23	30,42,50,52	0
3	EDO	B	8	4/4	0.90	0.12	4.42	29,32,39,41	0
3	EDO	C	10	4/4	0.85	0.22	3.11	35,37,42,51	0
4	FLC	C	12	13/13	0.85	0.21	3.08	9,30,41,56	13
4	FLC	A	502	13/13	0.84	0.19	2.42	19,41,49,61	0
4	FLC	B	501	13/13	0.77	0.18	2.40	33,41,48,49	13
3	EDO	A	1	4/4	0.84	0.19	2.29	33,34,39,40	0
3	EDO	C	9[B]	4/4	0.81	0.20	2.11	20,27,34,36	4
3	EDO	C	9[A]	4/4	0.81	0.20	2.11	27,29,31,35	4
4	FLC	A	501	13/13	0.91	0.15	2.01	30,42,47,49	0
4	FLC	C	500	13/13	0.89	0.17	1.37	20,40,57,60	0
3	EDO	D	12	4/4	0.94	0.10	1.03	24,30,31,34	0
2	LDN	A	3	31/31	0.95	0.11	0.59	11,19,37,58	0
3	EDO	D	13[A]	4/4	0.91	0.12	0.16	13,24,31,32	4
3	EDO	D	13[B]	4/4	0.91	0.12	0.13	21,27,33,42	4
3	EDO	C	11	4/4	0.90	0.11	-0.05	29,35,41,44	0
3	EDO	B	7	4/4	0.94	0.09	-0.06	19,29,36,41	0
2	LDN	C	4	31/31	0.95	0.09	-0.28	9,15,21,25	0
2	LDN	D	2	31/31	0.96	0.09	-0.38	12,18,49,55	0
2	LDN	B	1	31/31	0.96	0.08	-0.41	14,19,65,70	0
3	EDO	A	2	4/4	0.97	0.08	-0.57	22,25,27,30	0
3	EDO	D	6	4/4	0.66	0.23	-	31,38,40,48	0
3	EDO	A	5	4/4	0.81	0.15	-	32,35,37,49	0
3	EDO	A	4	4/4	0.82	0.30	-	32,34,35,42	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.