



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:38 PM GMT

PDB ID : 1PY2
Title : Structure of a 60 nM Small Molecule Bound to a Hot Spot on IL-2
Authors : Thanos, C.D.; Randal, M.; Wells, J.A.
Deposited on : 2003-07-07
Resolution : 2.80 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

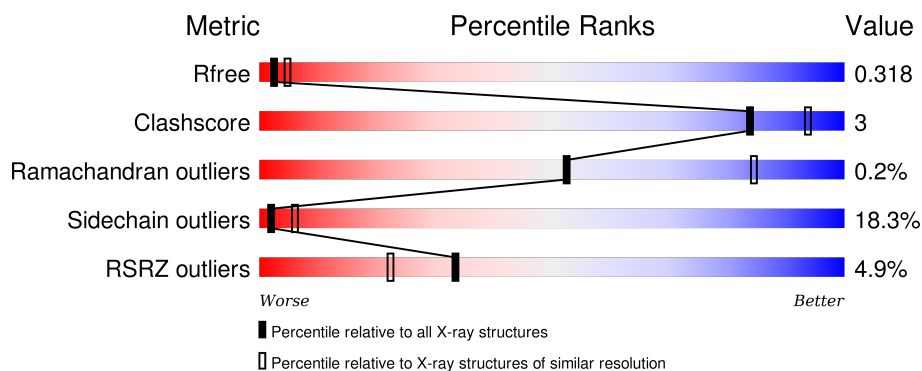
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 ≥ 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	132	<div> <div>4%</div> <div>64% 20% 5% 11%</div> </div>
1	B	132	<div> <div>2%</div> <div>58% 23% • • 12%</div> </div>
1	C	132	<div> <div>4%</div> <div>60% 21% 6% 13%</div> </div>
1	D	132	<div> <div>8%</div> <div>67% 20% • 9%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FRH	C	401	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4015 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.

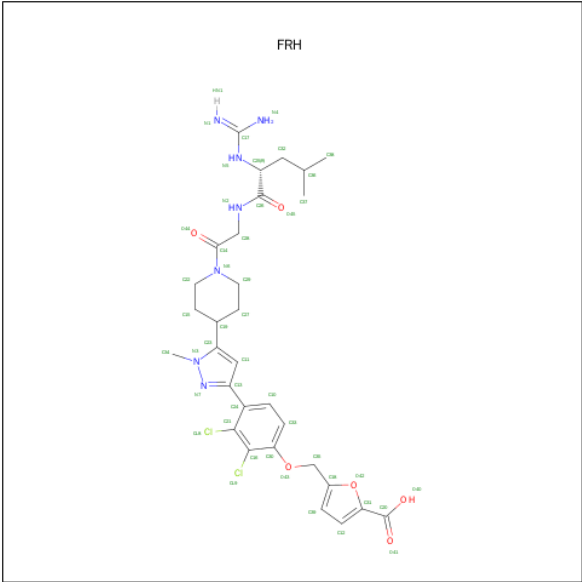
- Molecule 1 is a protein called Interleukin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	117	Total	C	N	O	S	50	0	0
			959	623	152	177	7			
1	B	116	Total	C	N	O	S	54	0	0
			951	616	154	174	7			
1	C	115	Total	C	N	O	S	48	0	0
			944	610	152	175	7			
1	D	120	Total	C	N	O	S	24	0	0
			978	631	158	182	7			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	C	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 5-[2,3-DICHLORO-4-(5-{1-[2-(2-GUANIDINO-4-METHYL-PENTANOYLAMINO)-ACETYL]-PIPERIDIN-4-YL}-1-METHYL-1H-PYRAZOL-3-YL)-PHE NOXYMETHYL]-FURAN-2-CARBOXYLIC ACID (three-letter code: FRH) (formula: C₃₀H₃₇Cl₂N₇O₆).

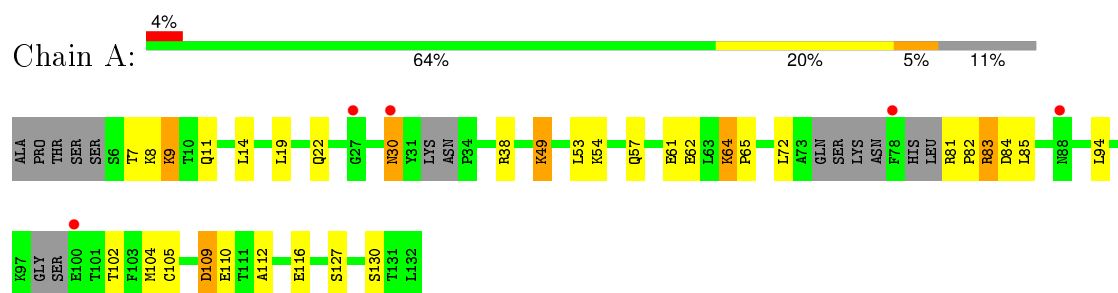


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			45	30	2	7	6		
3	B	1	Total	C	Cl	N	O	0	0
			45	30	2	7	6		
3	C	1	Total	C	Cl	N	O	0	0
			45	30	2	7	6		
3	D	1	Total	C	Cl	N	O	0	0
			45	30	2	7	6		

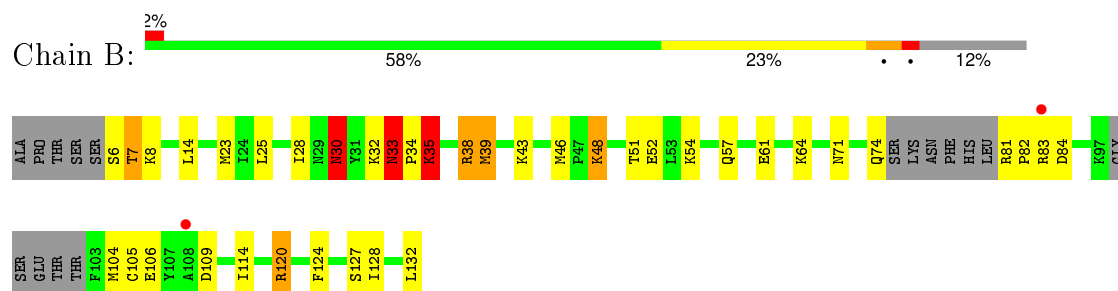
3 Residue-property plots [i](#)

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.

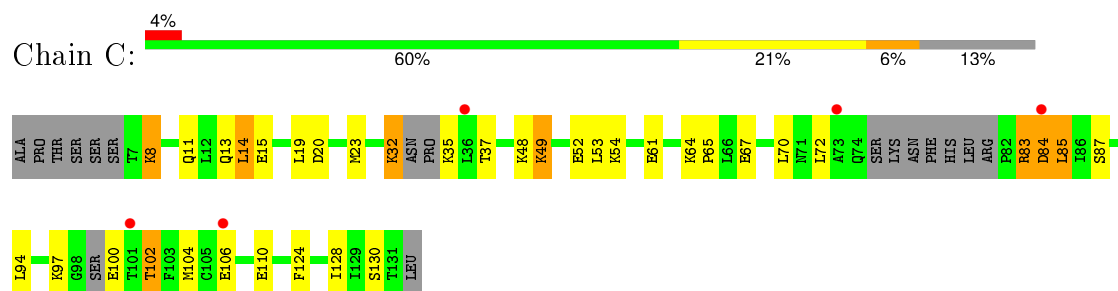
• Molecule 1: Interleukin-2



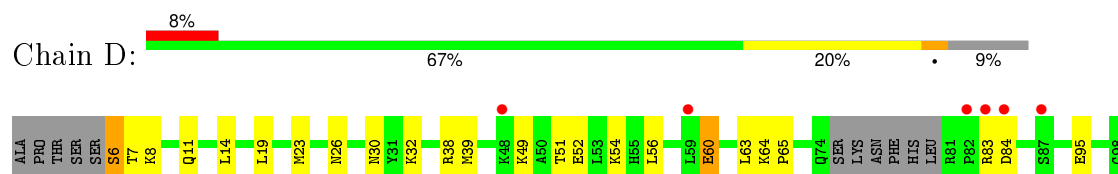
• Molecule 1: Interleukin-2

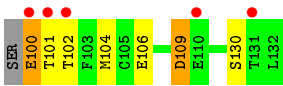


• Molecule 1: Interleukin-2



• Molecule 1: Interleukin-2





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.98Å 52.45Å 89.47Å 90.00° 106.34° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 19.90 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.4 (15.00-2.80) 98.4 (19.90-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.271 , 0.320 0.265 , 0.318	Depositor DCC
R_{free} test set	656 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	57.5	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 13135 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4015	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.99% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, FRH

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	2.16	10/971 (1.0%)	1.38	16/1306 (1.2%)
1	B	2.90	11/964 (1.1%)	1.38	17/1299 (1.3%)
1	C	1.89	13/955 (1.4%)	1.09	15/1283 (1.2%)
1	D	1.67	7/991 (0.7%)	1.42	11/1336 (0.8%)
All	All	2.20	41/3881 (1.1%)	1.33	59/5224 (1.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	32	LYS	CB-CG	75.71	3.56	1.52
1	A	49	LYS	CB-CG	42.04	2.66	1.52
1	C	83	ARG	CB-CG	39.77	2.60	1.52
1	D	102	THR	CB-OG1	29.05	2.01	1.43
1	B	64	LYS	CB-CG	26.30	2.23	1.52
1	A	30	ASN	CG-OD1	24.89	1.78	1.24
1	A	130	SER	CB-OG	-24.70	1.10	1.42
1	D	8	LYS	CB-CG	24.15	2.17	1.52
1	A	127	SER	CB-OG	-23.09	1.12	1.42
1	B	30	ASN	CB-CG	21.79	2.01	1.51
1	D	52	GLU	CB-CG	-20.73	1.12	1.52
1	D	11	GLN	CB-CG	19.20	2.04	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	104	MET	CB-CG	19.03	2.12	1.51
1	C	110	GLU	CB-CG	18.79	1.87	1.52
1	C	37	THR	CB-OG1	16.85	1.76	1.43
1	A	83	ARG	CB-CG	-16.76	1.07	1.52
1	D	8	LYS	CD-CE	15.34	1.89	1.51
1	B	7	THR	CA-CB	15.03	1.92	1.53
1	C	83	ARG	C-N	-14.77	1.00	1.34
1	A	94	LEU	CB-CG	-13.64	1.12	1.52
1	C	100	GLU	CB-CG	-12.27	1.28	1.52
1	C	84	ASP	C-N	-12.05	1.06	1.34
1	C	49	LYS	CG-CD	11.91	1.93	1.52
1	A	7	THR	CB-CG2	11.57	1.90	1.52
1	B	35	LYS	CB-CG	-11.50	1.21	1.52
1	A	8	LYS	CB-CG	-11.02	1.22	1.52
1	C	8	LYS	CD-CE	10.90	1.78	1.51
1	A	64	LYS	CB-CG	-10.34	1.24	1.52
1	D	100	GLU	CB-CG	-10.20	1.32	1.52
1	D	6	SER	CA-CB	-9.80	1.38	1.52
1	B	71	ASN	CB-CG	-9.40	1.29	1.51
1	C	35	LYS	CB-CG	8.95	1.76	1.52
1	B	33	ASN	CB-CG	8.90	1.71	1.51
1	B	74	GLN	CB-CG	8.72	1.76	1.52
1	C	32	LYS	CB-CG	8.09	1.74	1.52
1	C	54	LYS	CB-CG	-7.91	1.31	1.52
1	C	52	GLU	CB-CG	-7.54	1.37	1.52
1	C	85	LEU	N-CA	5.92	1.58	1.46
1	B	64	LYS	CA-CB	-5.61	1.41	1.53
1	B	57	GLN	CB-CG	5.47	1.67	1.52
1	A	85	LEU	CB-CG	5.31	1.68	1.52

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	100	GLU	CA-CB-CG	-24.01	60.58	113.40
1	D	8	LYS	CD-CE-NZ	-23.80	56.95	111.70
1	B	32	LYS	CA-CB-CG	-22.94	62.94	113.40
1	A	8	LYS	CA-CB-CG	-19.00	71.60	113.40
1	B	7	THR	N-CA-CB	16.98	142.57	110.30
1	A	9	LYS	CG-CD-CE	16.02	159.97	111.90
1	B	33	ASN	CB-CG-OD1	-15.13	91.34	121.60
1	D	8	LYS	CB-CG-CD	15.09	150.84	111.60
1	A	8	LYS	CB-CG-CD	-15.05	72.47	111.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	100	GLU	CB-CG-CD	-14.54	74.94	114.20
1	B	64	LYS	CB-CG-CD	-13.48	76.55	111.60
1	A	30	ASN	OD1-CG-ND2	-13.37	91.16	121.90
1	D	8	LYS	CG-CD-CE	-13.30	72.01	111.90
1	C	37	THR	CA-CB-CG2	-13.14	94.00	112.40
1	B	48	LYS	CA-CB-CG	12.83	141.63	113.40
1	A	30	ASN	CB-CG-OD1	-12.79	96.03	121.60
1	A	49	LYS	CA-CB-CG	-12.68	85.50	113.40
1	D	102	THR	OG1-CB-CG2	-11.97	82.48	110.00
1	B	33	ASN	CB-CG-ND2	11.72	144.83	116.70
1	C	83	ARG	CA-CB-CG	-11.59	87.91	113.40
1	A	64	LYS	CA-CB-CG	11.53	138.77	113.40
1	A	94	LEU	CB-CG-CD2	-11.20	91.97	111.00
1	A	9	LYS	CD-CE-NZ	11.16	137.37	111.70
1	C	37	THR	CA-CB-OG1	-10.82	86.28	109.00
1	D	104	MET	CA-CB-CG	-10.38	95.66	113.30
1	A	7	THR	OG1-CB-CG2	-10.14	86.68	110.00
1	B	7	THR	CA-CB-CG2	10.13	126.58	112.40
1	D	8	LYS	CA-CB-CG	-9.49	92.53	113.40
1	D	6	SER	N-CA-CB	9.20	124.30	110.50
1	C	85	LEU	N-CA-C	-9.00	86.71	111.00
1	B	30	ASN	CA-CB-CG	8.84	132.84	113.40
1	C	32	LYS	CA-CB-CG	-8.65	94.37	113.40
1	C	37	THR	OG1-CB-CG2	-8.52	90.41	110.00
1	C	84	ASP	O-C-N	-8.39	109.28	122.70
1	C	83	ARG	O-C-N	7.35	134.46	122.70
1	C	52	GLU	CA-CB-CG	-7.09	97.80	113.40
1	B	106	GLU	CB-CG-CD	-7.05	95.17	114.20
1	B	71	ASN	CA-CB-CG	6.41	127.50	113.40
1	C	85	LEU	N-CA-CB	6.35	123.09	110.40
1	A	7	THR	CA-CB-CG2	-6.13	103.82	112.40
1	C	84	ASP	CA-C-N	5.89	130.17	117.20
1	C	100	GLU	CA-CB-CG	-5.75	100.76	113.40
1	B	30	ASN	CB-CG-ND2	-5.51	103.47	116.70
1	A	54	LYS	CA-CB-CG	-5.47	101.37	113.40
1	C	83	ARG	CA-C-N	-5.44	105.22	117.20
1	A	64	LYS	CB-CG-CD	-5.43	97.47	111.60
1	A	109	ASP	CB-CG-OD2	5.33	123.09	118.30
1	B	84	ASP	CB-CG-OD2	5.32	123.09	118.30
1	B	32	LYS	CB-CG-CD	-5.31	97.79	111.60
1	A	84	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	83	ARG	CG-CD-NE	-5.25	100.78	111.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	84	ASP	CB-CG-OD2	5.24	123.01	118.30
1	B	109	ASP	CB-CG-OD2	5.21	122.98	118.30
1	B	64	LYS	CA-CB-CG	-5.20	101.97	113.40
1	C	84	ASP	CB-CG-OD2	5.17	122.95	118.30
1	B	57	GLN	CA-CB-CG	-5.12	102.13	113.40
1	C	8	LYS	CG-CD-CE	-5.11	96.56	111.90
1	D	109	ASP	CB-CG-OD2	5.07	122.86	118.30
1	B	30	ASN	CB-CG-OD1	-5.04	111.52	121.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	30	ASN	Sidechain
1	B	30	ASN	Sidechain

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	959	0	988	3	2
1	B	951	0	987	12	4
1	C	944	0	979	4	2
1	D	978	0	1008	2	4
2	B	2	0	0	0	0
2	C	1	0	0	0	0
3	A	45	0	35	0	0
3	B	45	0	35	5	0
3	C	45	0	35	0	0
3	D	45	0	35	1	0
All	All	4015	0	4102	22	6

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 3.

All (22) 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:33:ASN:HB2	1:B:34:PRO:HD3	1.56	0.88
1:B:33:ASN:CB	1:B:34:PRO:HD3	2.21	0.70
1:B:33:ASN:HB2	1:B:34:PRO:CD	2.24	0.67
1:C:83:ARG:O	1:C:84:ASP:HB2	1.96	0.65
1:D:64:LYS:HB2	1:D:65:PRO:HD3	1.87	0.57
1:B:38:ARG:HD2	3:B:301:FRH:C33	2.40	0.51
1:A:112:ALA:HB1	1:A:116:GLU:HB3	1.93	0.50
1:B:35:LYS:NZ	3:B:301:FRH:H352	2.28	0.49
1:D:60:GLU:HA	1:D:63:LEU:HD12	1.96	0.47
1:C:64:LYS:HB3	1:C:65:PRO:HD3	1.97	0.46
1:C:124:PHE:O	1:C:128:ILE:HG12	2.17	0.45
1:B:46:MET:HE3	1:B:120:ARG:HH11	1.83	0.44
3:D:501:FRH:H281	3:D:501:FRH:H292	1.80	0.43
1:B:38:ARG:CD	3:B:301:FRH:C10	2.97	0.43
1:C:14:LEU:HD11	1:C:53:LEU:HD21	2.01	0.42
1:B:38:ARG:CD	3:B:301:FRH:C33	2.98	0.42
1:A:81:ARG:HA	1:A:82:PRO:HD3	1.88	0.41
1:A:62:GLU:C	1:A:65:PRO:HD2	2.40	0.41
1:B:81:ARG:HA	1:B:82:PRO:HD3	1.87	0.41
1:B:35:LYS:HZ1	3:B:301:FRH:H352	1.85	0.41
1:B:28:ILE:HG23	1:B:39:MET:HE1	2.02	0.40
1:B:124:PHE:O	1:B:128:ILE:HG12	2.21	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:LEU:CD2	1:D:100:GLU:OE2[2_646]	1.07	1.13
1:B:52:GLU:OE1	1:C:102:THR:OG1[2_656]	1.41	0.79
1:B:52:GLU:CD	1:C:102:THR:OG1[2_656]	2.01	0.19
1:A:72:LEU:CD2	1:D:100:GLU:CD[2_646]	2.11	0.09
1:B:8:LYS:NZ	1:D:26:ASN:OD1[1_655]	2.16	0.04
1:B:8:LYS:CE	1:D:26:ASN:OD1[1_655]	2.17	0.03

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	108/132 (82%)	107 (99%)	1 (1%)	0	100	100
1	B	110/132 (83%)	107 (97%)	2 (2%)	1 (1%)	21	55
1	C	107/132 (81%)	105 (98%)	2 (2%)	0	100	100
1	D	114/132 (86%)	113 (99%)	1 (1%)	0	100	100
All	All	439/528 (83%)	432 (98%)	6 (1%)	1 (0%)	52	84

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	33	ASN

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	111/125 (89%)	94 (85%)	17 (15%)	3	10
1	B	110/125 (88%)	89 (81%)	21 (19%)	2	5
1	C	109/125 (87%)	86 (79%)	23 (21%)	1	4
1	D	113/125 (90%)	93 (82%)	20 (18%)	2	7
All	All	443/500 (89%)	362 (82%)	81 (18%)	2	6

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	11	GLN
1	A	14	LEU
1	A	19	LEU
1	A	22	GLN
1	A	38	ARG
1	A	49	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	53	LEU
1	A	57	GLN
1	A	61	GLU
1	A	64	LYS
1	A	83	ARG
1	A	102	THR
1	A	104	MET
1	A	105	CYS
1	A	109	ASP
1	A	110	GLU
1	B	6	SER
1	B	7	THR
1	B	14	LEU
1	B	23	MET
1	B	25	LEU
1	B	30	ASN
1	B	33	ASN
1	B	35	LYS
1	B	38	ARG
1	B	39	MET
1	B	43	LYS
1	B	48	LYS
1	B	51	THR
1	B	54	LYS
1	B	61	GLU
1	B	83	ARG
1	B	105	CYS
1	B	114	ILE
1	B	120	ARG
1	B	127	SER
1	B	132	LEU
1	C	8	LYS
1	C	11	GLN
1	C	13	GLN
1	C	14	LEU
1	C	15	GLU
1	C	19	LEU
1	C	20	ASP
1	C	23	MET
1	C	32	LYS
1	C	48	LYS
1	C	49	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	61	GLU
1	C	67	GLU
1	C	70	LEU
1	C	72	LEU
1	C	85	LEU
1	C	87	SER
1	C	94	LEU
1	C	97	LYS
1	C	102	THR
1	C	104	MET
1	C	106	GLU
1	C	130	SER
1	D	6	SER
1	D	7	THR
1	D	14	LEU
1	D	19	LEU
1	D	23	MET
1	D	30	ASN
1	D	32	LYS
1	D	38	ARG
1	D	39	MET
1	D	49	LYS
1	D	51	THR
1	D	54	LYS
1	D	56	LEU
1	D	60	GLU
1	D	83	ARG
1	D	95	GLU
1	D	101	THR
1	D	106	GLU
1	D	109	ASP
1	D	130	SER

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	90	ASN
1	A	126	GLN
1	B	22	GLN
1	C	90	ASN
1	D	22	GLN
1	D	71	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 7 ligands modelled in this entry, 3 are 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	FRH	A	201	-	39,48,48	2.30	8 (20%)	47,68,68	2.56	8 (17%)
3	FRH	B	301	-	39,48,48	2.29	8 (20%)	47,68,68	2.56	7 (14%)
3	FRH	C	401	-	39,48,48	2.30	8 (20%)	47,68,68	2.60	6 (12%)
3	FRH	D	501	-	39,48,48	2.32	8 (20%)	47,68,68	2.49	8 (17%)

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	FRH	A	201	-	-	0/29/48/48	0/3/4/4
3	FRH	B	301	-	-	0/29/48/48	0/3/4/4
3	FRH	C	401	-	-	0/29/48/48	0/3/4/4
3	FRH	D	501	-	-	0/29/48/48	0/3/4/4

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	FRH	C11-C13	-7.11	1.27	1.40
3	C	401	FRH	C11-C23	-6.93	1.26	1.38
3	D	501	FRH	C11-C13	-6.92	1.27	1.40
3	B	301	FRH	C11-C13	-6.91	1.27	1.40
3	A	201	FRH	C11-C13	-6.87	1.27	1.40
3	D	501	FRH	C11-C23	-6.80	1.27	1.38
3	A	201	FRH	N7-N3	-6.72	1.30	1.37
3	D	501	FRH	N7-N3	-6.71	1.30	1.37
3	B	301	FRH	C11-C23	-6.63	1.27	1.38
3	A	201	FRH	C11-C23	-6.63	1.27	1.38
3	B	301	FRH	N7-N3	-6.50	1.30	1.37
3	C	401	FRH	N7-N3	-6.23	1.31	1.37
3	A	201	FRH	C39-C18	-5.36	1.26	1.39
3	B	301	FRH	C39-C18	-5.36	1.26	1.39
3	D	501	FRH	C39-C18	-5.32	1.26	1.39
3	C	401	FRH	C39-C18	-5.28	1.27	1.39
3	D	501	FRH	C23-N3	-3.16	1.32	1.37
3	C	401	FRH	C23-N3	-2.90	1.33	1.37
3	A	201	FRH	C23-N3	-2.88	1.33	1.37
3	B	301	FRH	C23-N3	-2.84	1.33	1.37
3	C	401	FRH	C12-C39	-2.26	1.27	1.39
3	A	201	FRH	C12-C39	-2.25	1.27	1.39
3	D	501	FRH	C12-C39	-2.25	1.27	1.39
3	B	301	FRH	C12-C39	-2.24	1.27	1.39
3	A	201	FRH	C21-CL8	3.34	1.79	1.72
3	D	501	FRH	C16-CL9	3.35	1.79	1.72
3	C	401	FRH	C16-CL9	3.36	1.79	1.72
3	B	301	FRH	C16-CL9	3.39	1.80	1.72
3	C	401	FRH	C21-CL8	3.40	1.80	1.72
3	A	201	FRH	C16-CL9	3.42	1.80	1.72
3	B	301	FRH	C21-CL8	3.43	1.80	1.72
3	D	501	FRH	C21-CL8	3.44	1.80	1.72

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	501	FRH	C15-C22-N6	-3.46	106.06	111.07
3	C	401	FRH	C27-C29-N6	-3.42	106.11	111.07
3	C	401	FRH	C15-C22-N6	-3.35	106.22	111.07
3	D	501	FRH	C27-C29-N6	-2.74	107.09	111.07
3	D	501	FRH	O43-C30-C33	-2.69	118.38	124.01
3	B	301	FRH	C27-C29-N6	-2.62	107.28	111.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	201	FRH	C27-C29-N6	-2.49	107.46	111.07
3	A	201	FRH	C15-C22-N6	-2.43	107.56	111.07
3	B	301	FRH	C15-C22-N6	-2.11	108.02	111.07
3	A	201	FRH	C24-C21-CL8	2.09	121.38	119.72
3	B	301	FRH	C11-C13-C24	2.12	132.35	129.40
3	C	401	FRH	C35-O43-C30	2.23	122.23	117.82
3	A	201	FRH	C35-O43-C30	2.26	122.30	117.82
3	A	201	FRH	C11-C13-C24	2.31	132.60	129.40
3	C	401	FRH	C11-C23-C19	2.35	132.40	128.73
3	B	301	FRH	C35-O43-C30	2.66	123.10	117.82
3	D	501	FRH	C35-O43-C30	2.76	123.29	117.82
3	B	301	FRH	C11-C23-C19	2.89	133.24	128.73
3	A	201	FRH	C11-C23-C19	3.08	133.54	128.73
3	D	501	FRH	C11-C23-C19	3.15	133.65	128.73
3	D	501	FRH	O43-C30-C16	3.49	122.11	115.84
3	D	501	FRH	C12-C39-C18	8.54	111.46	106.78
3	A	201	FRH	C12-C39-C18	9.94	112.22	106.78
3	B	301	FRH	C12-C39-C18	10.16	112.34	106.78
3	C	401	FRH	C12-C39-C18	11.17	112.90	106.78
3	D	501	FRH	C13-C11-C23	11.58	111.89	106.09
3	C	401	FRH	C13-C11-C23	11.61	111.90	106.09
3	A	201	FRH	C13-C11-C23	12.03	112.11	106.09
3	B	301	FRH	C13-C11-C23	12.08	112.14	106.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	301	FRH	5	0
3	D	501	FRH	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	117/132 (88%)	0.21	5 (4%) 39 27	29, 54, 86, 96	16 (13%)
1	B	116/132 (87%)	0.17	2 (1%) 73 63	34, 54, 83, 91	15 (12%)
1	C	115/132 (87%)	0.30	5 (4%) 39 27	28, 56, 89, 110	13 (11%)
1	D	120/132 (90%)	0.47	11 (9%) 11 5	37, 56, 78, 84	8 (6%)
All	All	468/528 (88%)	0.29	23 (4%) 33 22	28, 55, 84, 110	52 (11%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	102	THR	5.3
1	C	101	THR	4.5
1	D	100	GLU	4.4
1	A	30	ASN	4.3
1	D	110	GLU	4.2
1	D	101	THR	3.8
1	A	27	GLY	3.7
1	B	83	ARG	3.7
1	D	84	ASP	3.5
1	D	87	SER	3.4
1	D	83	ARG	3.2
1	C	73	ALA	3.1
1	D	131	THR	2.9
1	A	88	ASN	2.9
1	A	100	GLU	2.7
1	C	84	ASP	2.6
1	C	36	LEU	2.5
1	A	78	PHE	2.4
1	D	48	LYS	2.2
1	D	59	LEU	2.2
1	C	106	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	108	ALA	2.0
1	D	82	PRO	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
3	FRH	C	401	45/45	0.68	0.36	2.17	49,115,147,155	0
3	FRH	D	501	45/45	0.88	0.24	0.79	43,63,116,137	0
3	FRH	B	301	45/45	0.88	0.24	0.28	35,56,96,110	0
3	FRH	A	201	45/45	0.88	0.26	-0.01	35,55,106,127	0
2	ZN	B	601	1/1	0.84	0.36	-	116,116,116,116	0
2	ZN	C	701	1/1	0.85	0.42	-	137,137,137,137	0
2	ZN	B	801	1/1	0.40	0.35	-	155,155,155,155	0

6.5 Other polymers [i](#)

There are no such residues in this entry.