W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Jun 16, 2024 – 05:36 AM EDT

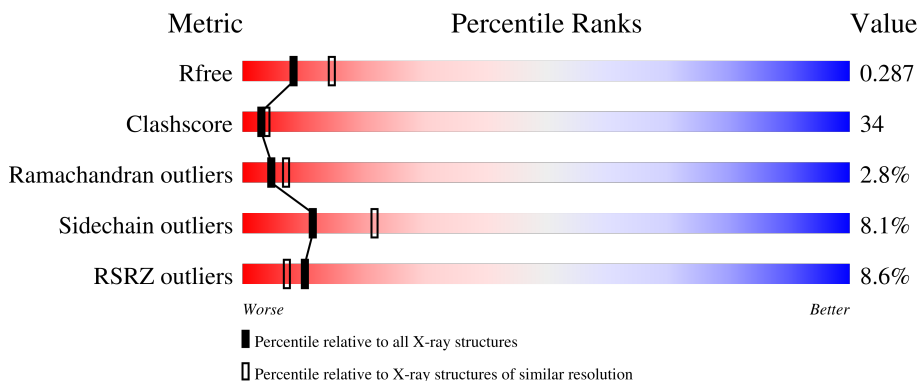|		
PDB ID	:	2OGJ
Title	:	Crystal structure of a dihydroorotase
Authors	:	Sugadev, R.; Kumaran, D.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2007-01-05
Resolution	:	2.62 Å(reported)

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 2.62 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	Percentile Ranks	Value
Rfree		0.287
Clashscore		34
Ramachandran outliers		2.8%
Sidechain outliers		8.1%
RSRZ outliers		8.6%

Worse　　　　　　　　　　　　　　　　　　　　*Better*

▮ Percentile relative to all X-ray structures
⬚ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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 <=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	417	2% / 57% 28% 6% 9%
1	B	417	2% / 52% 31% 5% · 12%
1	C	417	13% / 34% 36% 6% 24%
1	D	417	9% / 46% 37% · 13%
1	E	417	6% / 49% 34% 6% 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	417	10%　40%　38%　8%　14%

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
1	KCX	A	175	-	-	X	-
1	KCX	B	175	-	-	X	-
1	KCX	D	175	-	-	X	-
1	KCX	E	175	-	-	X	-
1	KCX	F	175	-	-	X	-

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 16585 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 Dihydroorotase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	379	Total	C	N	O	S	Se	0	0	0
			2876	1814	503	547	5	7			
1	B	369	Total	C	N	O	S	Se	0	0	0
			2809	1773	488	536	5	7			
1	C	317	Total	C	N	O	S	Se	0	0	0
			2433	1550	419	453	5	6			
1	D	364	Total	C	N	O	S	Se	0	0	0
			2782	1760	484	526	5	7			
1	E	372	Total	C	N	O	S	Se	0	0	0
			2822	1781	492	537	5	7			
1	F	359	Total	C	N	O	S	Se	0	0	0
			2728	1728	469	519	5	7			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	expression tag	UNP Q8UAV1
A	2	SER	-	expression tag	UNP Q8UAV1
A	3	LEU	-	expression tag	UNP Q8UAV1
A	410	GLU	-	expression tag	UNP Q8UAV1
A	411	GLY	-	expression tag	UNP Q8UAV1
A	412	HIS	-	expression tag	UNP Q8UAV1
A	413	HIS	-	expression tag	UNP Q8UAV1
A	414	HIS	-	expression tag	UNP Q8UAV1
A	415	HIS	-	expression tag	UNP Q8UAV1
A	416	HIS	-	expression tag	UNP Q8UAV1
A	417	HIS	-	expression tag	UNP Q8UAV1
B	1	MSE	-	expression tag	UNP Q8UAV1
B	2	SER	-	expression tag	UNP Q8UAV1
B	3	LEU	-	expression tag	UNP Q8UAV1
B	410	GLU	-	expression tag	UNP Q8UAV1
B	411	GLY	-	expression tag	UNP Q8UAV1
B	412	HIS	-	expression tag	UNP Q8UAV1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	413	HIS	-	expression tag	UNP Q8UAV1
B	414	HIS	-	expression tag	UNP Q8UAV1
B	415	HIS	-	expression tag	UNP Q8UAV1
B	416	HIS	-	expression tag	UNP Q8UAV1
B	417	HIS	-	expression tag	UNP Q8UAV1
C	1	MSE	-	expression tag	UNP Q8UAV1
C	2	SER	-	expression tag	UNP Q8UAV1
C	3	LEU	-	expression tag	UNP Q8UAV1
C	410	GLU	-	expression tag	UNP Q8UAV1
C	411	GLY	-	expression tag	UNP Q8UAV1
C	412	HIS	-	expression tag	UNP Q8UAV1
C	413	HIS	-	expression tag	UNP Q8UAV1
C	414	HIS	-	expression tag	UNP Q8UAV1
C	415	HIS	-	expression tag	UNP Q8UAV1
C	416	HIS	-	expression tag	UNP Q8UAV1
C	417	HIS	-	expression tag	UNP Q8UAV1
D	1	MSE	-	expression tag	UNP Q8UAV1
D	2	SER	-	expression tag	UNP Q8UAV1
D	3	LEU	-	expression tag	UNP Q8UAV1
D	410	GLU	-	expression tag	UNP Q8UAV1
D	411	GLY	-	expression tag	UNP Q8UAV1
D	412	HIS	-	expression tag	UNP Q8UAV1
D	413	HIS	-	expression tag	UNP Q8UAV1
D	414	HIS	-	expression tag	UNP Q8UAV1
D	415	HIS	-	expression tag	UNP Q8UAV1
D	416	HIS	-	expression tag	UNP Q8UAV1
D	417	HIS	-	expression tag	UNP Q8UAV1
E	1	MSE	-	expression tag	UNP Q8UAV1
E	2	SER	-	expression tag	UNP Q8UAV1
E	3	LEU	-	expression tag	UNP Q8UAV1
E	410	GLU	-	expression tag	UNP Q8UAV1
E	411	GLY	-	expression tag	UNP Q8UAV1
E	412	HIS	-	expression tag	UNP Q8UAV1
E	413	HIS	-	expression tag	UNP Q8UAV1
E	414	HIS	-	expression tag	UNP Q8UAV1
E	415	HIS	-	expression tag	UNP Q8UAV1
E	416	HIS	-	expression tag	UNP Q8UAV1
E	417	HIS	-	expression tag	UNP Q8UAV1
F	1	MSE	-	expression tag	UNP Q8UAV1
F	2	SER	-	expression tag	UNP Q8UAV1
F	3	LEU	-	expression tag	UNP Q8UAV1
F	410	GLU	-	expression tag	UNP Q8UAV1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	411	GLY	-	expression tag	UNP Q8UAV1
F	412	HIS	-	expression tag	UNP Q8UAV1
F	413	HIS	-	expression tag	UNP Q8UAV1
F	414	HIS	-	expression tag	UNP Q8UAV1
F	415	HIS	-	expression tag	UNP Q8UAV1
F	416	HIS	-	expression tag	UNP Q8UAV1
F	417	HIS	-	expression tag	UNP Q8UAV1

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Zn 2	0	0
2	B	2	Total 2	Zn 2	0	0
2	C	2	Total 2	Zn 2	0	0
2	D	2	Total 2	Zn 2	0	0
2	E	2	Total 2	Zn 2	0	0
2	F	2	Total 2	Zn 2	0	0

- Molecule 3 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).
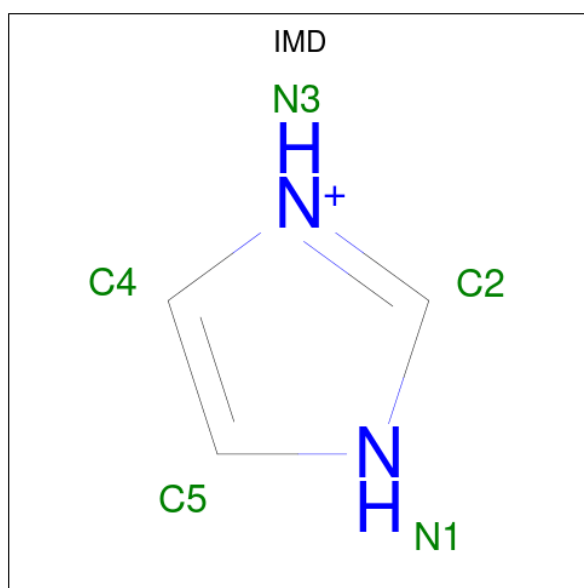
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total 5	C 3	N 2	0	0
3	D	1	Total 5	C 3	N 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	27	Total 27	O 27	0	0
4	B	26	Total 26	O 26	0	0
4	C	10	Total 10	O 10	0	0
4	D	13	Total 13	O 13	0	0
4	E	21	Total 21	O 21	0	0
4	F	16	Total 16	O 16	0	0

3   Residue-property plots ⓘ

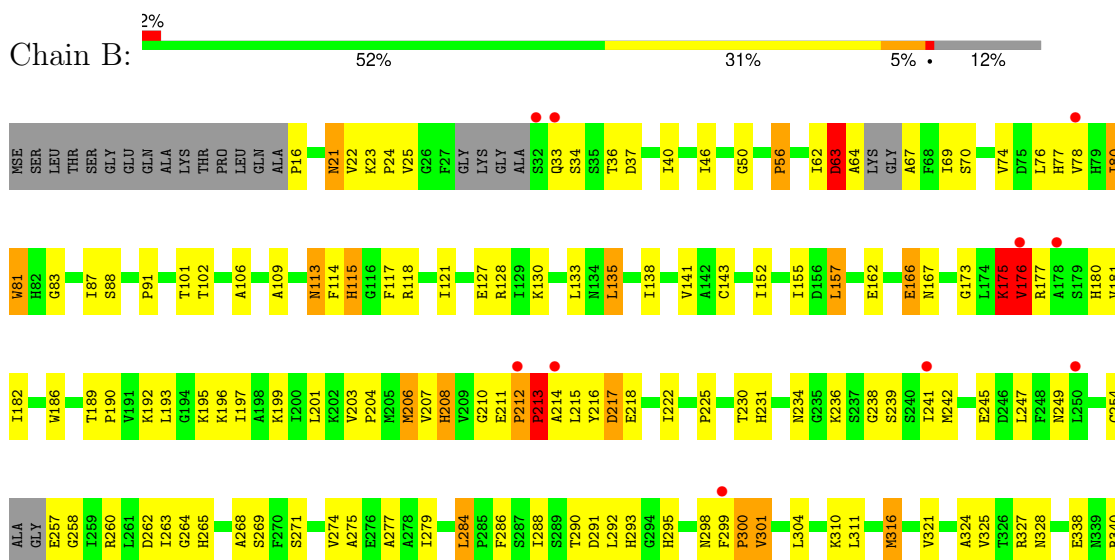These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Dihydroorotase

- Molecule 1: Dihydroorotase

• Molecule 1: Dihydroorotase

Chain C:

• Molecule 1: Dihydroorotase

Chain D:

ARG ALA ARG LYS LEU VAL ARG HIS SER HIS GLY TYR SER TRP ARG GLU GLY HIS HIS HIS HIS HIS

- Molecule 1: Dihydroorotase

Chain E:

6%

49% 34% 6% 11%

- Molecule 1: Dihydroorotase

Chain F:

10%

40% 38% 8% 14%
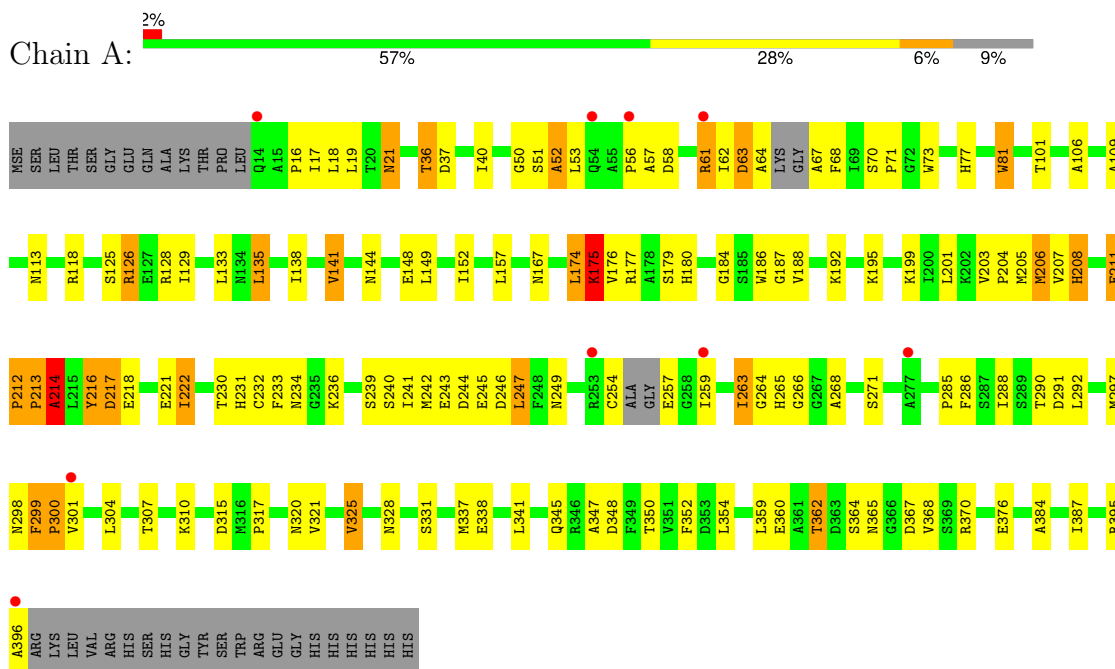
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	90.65Å 139.20Å 206.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.76 – 2.62 39.76 – 2.62	Depositor EDS
% Data completeness (in resolution range)	92.3 (39.76-2.62) 96.1 (39.76-2.62)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.98 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.256 , 0.302 0.243 , 0.287	Depositor DCC
R_{free} test set	4173 reflections (2.81%)	wwPDB-VP
Wilson B-factor (Å^2)	58.7	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 54.2	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	16585	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: ZN, IMD, KCX

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z| >5$	RMSZ	#$|Z| >5$
1	A	0.53	3/2910 (0.1%)	0.75	1/3932 (0.0%)
1	B	0.54	3/2841 (0.1%)	0.74	1/3837 (0.0%)
1	C	0.46	1/2461 (0.0%)	0.67	0/3322
1	D	0.50	2/2810 (0.1%)	0.72	0/3787
1	E	0.53	3/2854 (0.1%)	0.85	3/3856 (0.1%)
1	F	0.48	1/2757 (0.0%)	0.71	0/3721
All	All	0.51	13/16633 (0.1%)	0.74	5/22455 (0.0%)

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	2
1	E	0	2
All	All	0	5

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	63	ASP	C-N	-8.42	1.14	1.34
1	D	206	MSE	SE-CE	-6.25	1.58	1.95
1	B	176	VAL	C-N	6.10	1.48	1.34
1	B	316	MSE	SE-CE	-6.02	1.59	1.95
1	F	206	MSE	SE-CE	-5.84	1.60	1.95

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	63	ASP	O-C-N	-22.60	86.54	122.70
1	E	63	ASP	CA-C-N	16.26	152.97	117.20
1	E	63	ASP	C-N-CA	9.45	145.32	121.70
1	B	115	HIS	N-CA-C	-5.38	96.48	111.00
1	A	214	ALA	N-CA-C	-5.15	97.10	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	175	KCX	Mainchain
1	B	175	KCX	Mainchain
1	B	176	VAL	Mainchain
1	E	173	GLY	Mainchain
1	E	63	ASP	Peptide

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	2876	0	2862	156	0
1	B	2809	0	2788	185	0
1	C	2433	0	2411	215	0
1	D	2782	0	2771	181	3
1	E	2822	0	2796	168	3
1	F	2728	0	2704	249	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	C	5	0	4	0	0
3	D	5	0	4	0	0
4	A	27	0	0	2	0
4	B	26	0	0	1	0
4	C	10	0	0	1	0
4	D	13	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	21	0	0	1	0
4	F	16	0	0	0	0
All	All	16585	0	16340	1111	3

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 34.

The worst 5 of 1111 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:E:64:ALA:CB	1:E:67:ALA:HB2	1.57	1.32
1:A:317:PRO:HG2	1:A:320:ASN:HD22	1.00	1.17
1:F:17:ILE:CG2	1:F:40:ILE:HB	1.76	1.16
1:B:288:ILE:HD11	1:B:316:MSE:HE1	1.29	1.13
1:E:64:ALA:HB1	1:E:67:ALA:HB2	1.19	1.11

All (3) 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:D:225:PRO:CB	1:E:29:LYS:CD[1_655]	1.55	0.65
1:D:225:PRO:CB	1:E:29:LYS:CG[1_655]	1.70	0.50
1:D:225:PRO:CB	1:E:29:LYS:CE[1_655]	2.10	0.10

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	372/417 (89%)	330 (89%)	34 (9%)	8 (2%)	6	11
1	B	360/417 (86%)	314 (87%)	38 (11%)	8 (2%)	6	11

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	302/417 (72%)	245 (81%)	47 (16%)	10 (3%)	4	5
1	D	349/417 (84%)	308 (88%)	33 (10%)	8 (2%)	6	10
1	E	363/417 (87%)	306 (84%)	47 (13%)	10 (3%)	5	7
1	F	346/417 (83%)	294 (85%)	37 (11%)	15 (4%)	2	3
All	All	2092/2502 (84%)	1797 (86%)	236 (11%)	59 (3%)	5	7

5 of 59 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	PRO
1	A	212	PRO
1	A	214	ALA
1	D	212	PRO
1	D	214	ALA

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	306/329 (93%)	281 (92%)	25 (8%)	11	21
1	B	301/329 (92%)	281 (93%)	20 (7%)	16	32
1	C	260/329 (79%)	235 (90%)	25 (10%)	8	15
1	D	298/329 (91%)	283 (95%)	15 (5%)	24	46
1	E	300/329 (91%)	275 (92%)	25 (8%)	11	21
1	F	292/329 (89%)	260 (89%)	32 (11%)	6	10
All	All	1757/1974 (89%)	1615 (92%)	142 (8%)	11	22

5 of 142 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	65	LYS
1	F	135	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	247	LEU
1	C	81	TRP
1	C	61	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	21	ASN
1	E	60	GLN
1	F	365	ASN
1	D	33	GLN
1	D	180	HIS

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

5.4   Non-standard residues in protein, DNA, RNA chains ⓘ

6 non-standard protein/DNA/RNA residues 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	$\#|Z| > 2$
1	KCX	F	175	2,1	10,11,12	0.80	0	6,12,14	2.78	2 (33%)
1	KCX	B	175	2,1	10,11,12	0.79	0	6,12,14	2.79	2 (33%)
1	KCX	C	175	2,1	10,11,12	0.79	0	6,12,14	2.78	2 (33%)
1	KCX	A	175	2,1	10,11,12	0.79	0	6,12,14	2.78	2 (33%)
1	KCX	E	175	2,1	10,11,12	0.80	0	6,12,14	2.78	2 (33%)
1	KCX	D	175	2,1	10,11,12	0.79	0	6,12,14	2.76	2 (33%)

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
1	KCX	F	175	2,1	-	3/9/10/12	-
1	KCX	B	175	2,1	-	3/9/10/12	-
1	KCX	C	175	2,1	-	3/9/10/12	-
1	KCX	A	175	2,1	-	3/9/10/12	-
1	KCX	E	175	2,1	-	3/9/10/12	-
1	KCX	D	175	2,1	-	3/9/10/12	-

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	175	KCX	CE-NZ-CX	-6.26	111.36	121.98
1	C	175	KCX	CE-NZ-CX	-6.25	111.38	121.98
1	E	175	KCX	CE-NZ-CX	-6.25	111.38	121.98
1	F	175	KCX	CE-NZ-CX	-6.24	111.39	121.98
1	A	175	KCX	CE-NZ-CX	-6.24	111.39	121.98

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	175	KCX	OQ1-CX-NZ-CE
1	A	175	KCX	OQ2-CX-NZ-CE
1	B	175	KCX	OQ1-CX-NZ-CE
1	B	175	KCX	OQ2-CX-NZ-CE
1	C	175	KCX	OQ1-CX-NZ-CE

There are no ring outliers.

6 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	175	KCX	7	0
1	B	175	KCX	8	0
1	C	175	KCX	4	0
1	A	175	KCX	13	0
1	E	175	KCX	7	0
1	D	175	KCX	7	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 12 are monoatomic - leaving 2 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	IMD	C	3744	2	3,5,5	0.72	0	4,5,5	0.55	0
3	IMD	D	3745	2	3,5,5	0.70	0	4,5,5	0.62	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	IMD	C	3744	2	-	-	0/1/1/1
3	IMD	D	3745	2	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	E	2
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	174:LEU	C	175:KCX	N	1.70
1	E	174:LEU	C	175:KCX	N	1.60
1	E	63:ASP	C	64:ALA	N	1.14

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(Å²)	Q<0.9
1	A	371/417 (88%)	0.07	9 (2%)	59	53	32, 50, 72, 89	0
1	B	361/417 (86%)	0.22	10 (2%)	53	47	30, 54, 79, 90	0
1	C	310/417 (74%)	0.95	56 (18%)	1	0	48, 74, 96, 99	0
1	D	356/417 (85%)	0.36	38 (10%)	6	4	39, 60, 89, 99	0
1	E	364/417 (87%)	0.46	26 (7%)	16	11	35, 60, 80, 91	0
1	F	351/417 (84%)	0.59	42 (11%)	4	2	39, 66, 88, 99	0
All	All	2113/2502 (84%)	0.43	181 (8%)	10	7	30, 60, 87, 99	0

The worst 5 of 181 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	373	ARG	10.2
1	F	62	ILE	9.1
1	C	315	ASP	6.8
1	C	61	ARG	6.6
1	C	384	ALA	6.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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(Å²)	Q<0.9
1	KCX	B	175	12/13	0.81	0.30	48,52,64,65	0
1	KCX	A	175	12/13	0.82	0.30	36,45,70,72	0
1	KCX	E	175	12/13	0.84	0.23	48,57,74,77	0
1	KCX	D	175	12/13	0.85	0.22	47,53,71,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
1	KCX	C	175	12/13	0.85	0.26	62,65,76,78	0
1	KCX	F	175	12/13	0.87	0.23	47,52,73,75	0

6.3   Carbohydrates ⓘ

There are no monosaccharides 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. 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(Å²)	Q<0.9
2	ZN	C	601	1/1	0.77	0.07	87,87,87,87	0
2	ZN	E	801	1/1	0.83	0.10	86,86,86,86	0
2	ZN	D	701	1/1	0.86	0.05	71,71,71,71	0
2	ZN	D	700	1/1	0.88	0.10	60,60,60,60	0
2	ZN	F	901	1/1	0.89	0.05	83,83,83,83	0
2	ZN	F	900	1/1	0.91	0.10	58,58,58,58	0
3	IMD	D	3745	5/5	0.91	0.19	61,61,61,62	0
2	ZN	C	600	1/1	0.94	0.09	65,65,65,65	0
2	ZN	A	419	1/1	0.95	0.06	60,60,60,60	0
2	ZN	B	500	1/1	0.95	0.09	53,53,53,53	0
3	IMD	C	3744	5/5	0.96	0.14	69,69,69,70	0
2	ZN	E	800	1/1	0.96	0.14	59,59,59,59	0
2	ZN	A	418	1/1	0.97	0.07	42,42,42,42	0
2	ZN	B	501	1/1	0.97	0.11	73,73,73,73	0

6.5   Other polymers ⓘ

There are no such residues in this entry.