wwPDB X-ray Structure Validation Summary Report (i)

Oct 12, 2021 – 02:38 PM EDT

PDB ID	:	1ZXE
Title	:	Crystal Structure of eIF2alpha Protein Kinase GCN2: D835N Inactivating Mutant in Apo Form
Authors	:	Padyana, A.K.; Qiu, H.; Roll-Mecak, A.; Hinnebusch, A.G.; Burley, S.K.
Deposited on	:	2005-06-07
Resolution	:	2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

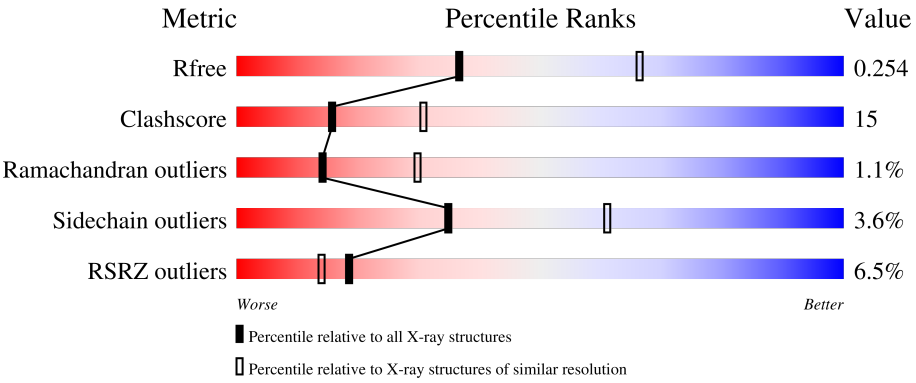
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	303	63% 25% 11%
1	B	303	5% 64% 18% 17%
1	C	303	4% 69% 20% 9%
1	D	303	4% 57% 25% 16%
1	E	303	11% 54% 31% 13%

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Mol	Chain	Length	Quality of chain
1	F	303	7% 52% 27% 18%

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
2	GOL	A	398	-	X	-	-
2	GOL	B	498	-	X	-	-
2	GOL	C	998	-	X	-	-
2	GOL	D	698	-	X	-	-
2	GOL	E	998	-	X	-	-
2	GOL	F	998	-	X	-	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 13242 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 Serine/threonine-protein kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	Se	0	0	0
			2222	1427	387	399	1	8			
1	B	252	Total	C	N	O	S	Se	0	0	0
			2081	1336	363	373	1	8			
1	C	275	Total	C	N	O	S	Se	0	0	0
			2259	1448	393	409	1	8			
1	D	256	Total	C	N	O	S	Se	0	0	0
			2117	1358	370	380	1	8			
1	E	264	Total	C	N	O	S	Se	0	0	0
			2181	1399	381	392	1	8			
1	F	249	Total	C	N	O	S	Se	0	0	0
			2067	1328	358	372	1	8			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	592	SER	-	cloning artifact	UNP P15442
A	593	LEU	-	cloning artifact	UNP P15442
A	645	MSE	MET	modified residue	UNP P15442
A	775	MSE	MET	modified residue	UNP P15442
A	788	MSE	MET	modified residue	UNP P15442
A	835	ASN	ASP	engineered mutation	UNP P15442
A	839	MSE	MET	modified residue	UNP P15442
A	889	MSE	MET	modified residue	UNP P15442
A	908	MSE	MET	modified residue	UNP P15442
A	918	MSE	MET	modified residue	UNP P15442
A	926	MSE	MET	modified residue	UNP P15442
A	951	MSE	MET	modified residue	UNP P15442
B	592	SER	-	cloning artifact	UNP P15442
B	593	LEU	-	cloning artifact	UNP P15442
B	645	MSE	MET	modified residue	UNP P15442
B	775	MSE	MET	modified residue	UNP P15442
B	788	MSE	MET	modified residue	UNP P15442

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Chain	Residue	Modelled	Actual	Comment	Reference
B	835	ASN	ASP	engineered mutation	UNP P15442
B	839	MSE	MET	modified residue	UNP P15442
B	889	MSE	MET	modified residue	UNP P15442
B	908	MSE	MET	modified residue	UNP P15442
B	918	MSE	MET	modified residue	UNP P15442
B	926	MSE	MET	modified residue	UNP P15442
B	951	MSE	MET	modified residue	UNP P15442
C	592	SER	-	cloning artifact	UNP P15442
C	593	LEU	-	cloning artifact	UNP P15442
C	645	MSE	MET	modified residue	UNP P15442
C	775	MSE	MET	modified residue	UNP P15442
C	788	MSE	MET	modified residue	UNP P15442
C	835	ASN	ASP	engineered mutation	UNP P15442
C	839	MSE	MET	modified residue	UNP P15442
C	889	MSE	MET	modified residue	UNP P15442
C	908	MSE	MET	modified residue	UNP P15442
C	918	MSE	MET	modified residue	UNP P15442
C	926	MSE	MET	modified residue	UNP P15442
C	951	MSE	MET	modified residue	UNP P15442
D	592	SER	-	cloning artifact	UNP P15442
D	593	LEU	-	cloning artifact	UNP P15442
D	645	MSE	MET	modified residue	UNP P15442
D	775	MSE	MET	modified residue	UNP P15442
D	788	MSE	MET	modified residue	UNP P15442
D	835	ASN	ASP	engineered mutation	UNP P15442
D	839	MSE	MET	modified residue	UNP P15442
D	889	MSE	MET	modified residue	UNP P15442
D	908	MSE	MET	modified residue	UNP P15442
D	918	MSE	MET	modified residue	UNP P15442
D	926	MSE	MET	modified residue	UNP P15442
D	951	MSE	MET	modified residue	UNP P15442
E	592	SER	-	cloning artifact	UNP P15442
E	593	LEU	-	cloning artifact	UNP P15442
E	645	MSE	MET	modified residue	UNP P15442
E	775	MSE	MET	modified residue	UNP P15442
E	788	MSE	MET	modified residue	UNP P15442
E	835	ASN	ASP	engineered mutation	UNP P15442
E	839	MSE	MET	modified residue	UNP P15442
E	889	MSE	MET	modified residue	UNP P15442
E	908	MSE	MET	modified residue	UNP P15442
E	918	MSE	MET	modified residue	UNP P15442
E	926	MSE	MET	modified residue	UNP P15442

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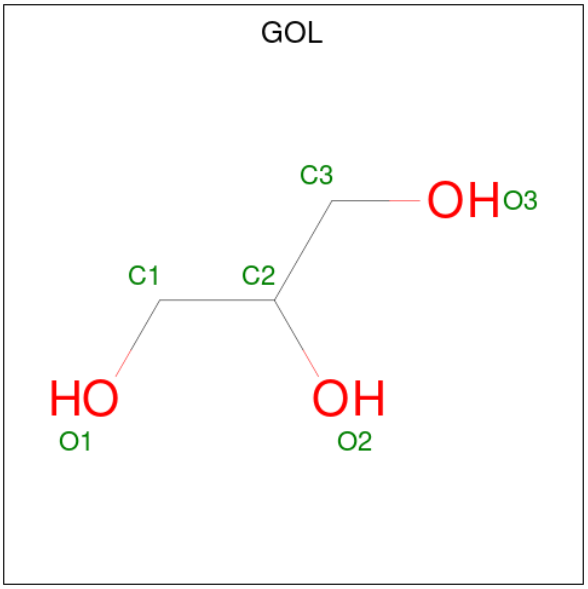
Chain	Residue	Modelled	Actual	Comment	Reference
E	951	MSE	MET	modified residue	UNP P15442
F	592	SER	-	cloning artifact	UNP P15442
F	593	LEU	-	cloning artifact	UNP P15442
F	645	MSE	MET	modified residue	UNP P15442
F	775	MSE	MET	modified residue	UNP P15442
F	788	MSE	MET	modified residue	UNP P15442
F	835	ASN	ASP	engineered mutation	UNP P15442
F	839	MSE	MET	modified residue	UNP P15442
F	889	MSE	MET	modified residue	UNP P15442
F	908	MSE	MET	modified residue	UNP P15442
F	918	MSE	MET	modified residue	UNP P15442
F	926	MSE	MET	modified residue	UNP P15442
F	951	MSE	MET	modified residue	UNP P15442

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is water.

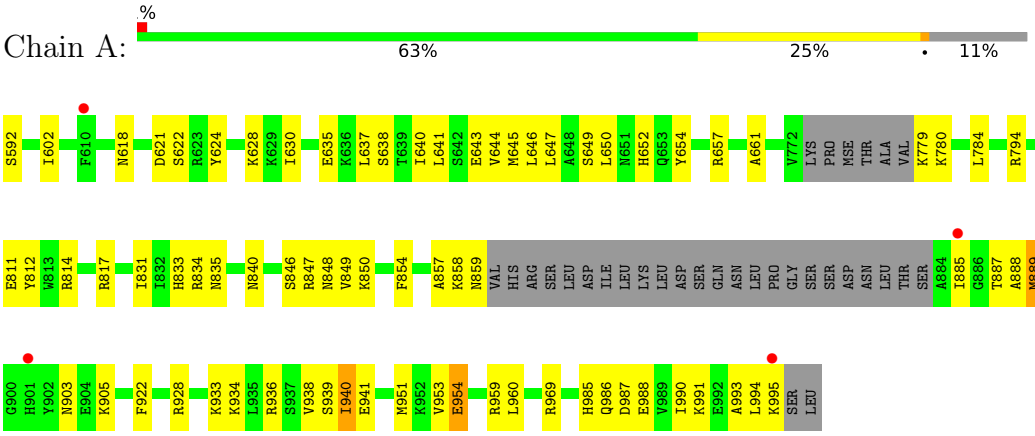
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	67	Total	O	0	0
			67	67		
3	B	51	Total	O	0	0
			51	51		
3	C	57	Total	O	0	0
			57	57		
3	D	72	Total	O	0	0
			72	72		
3	E	11	Total	O	0	0
			11	11		
3	F	21	Total	O	0	0
			21	21		

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.

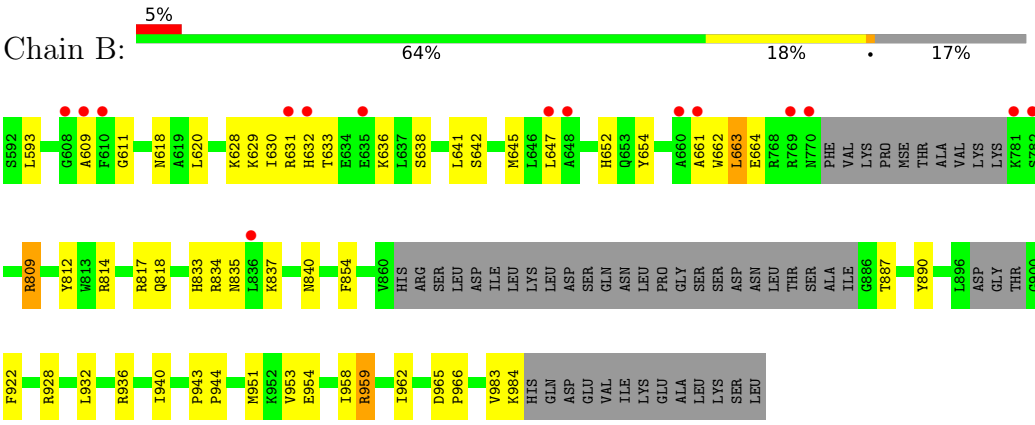
• Molecule 1: Serine/threonine-protein kinase

Chain A:



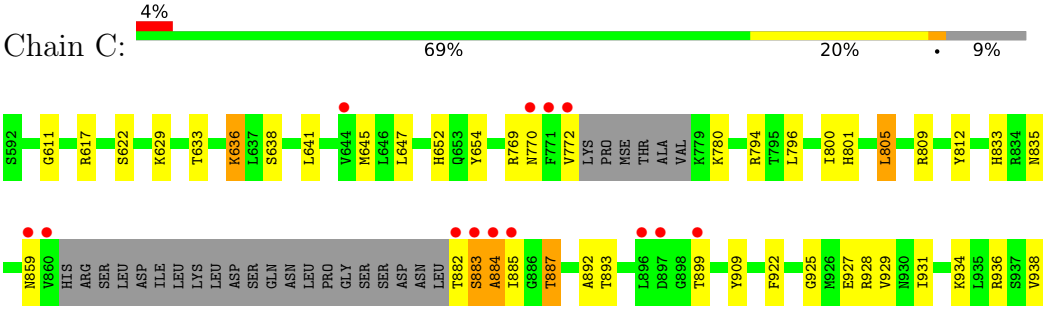
• Molecule 1: Serine/threonine-protein kinase

Chain B:



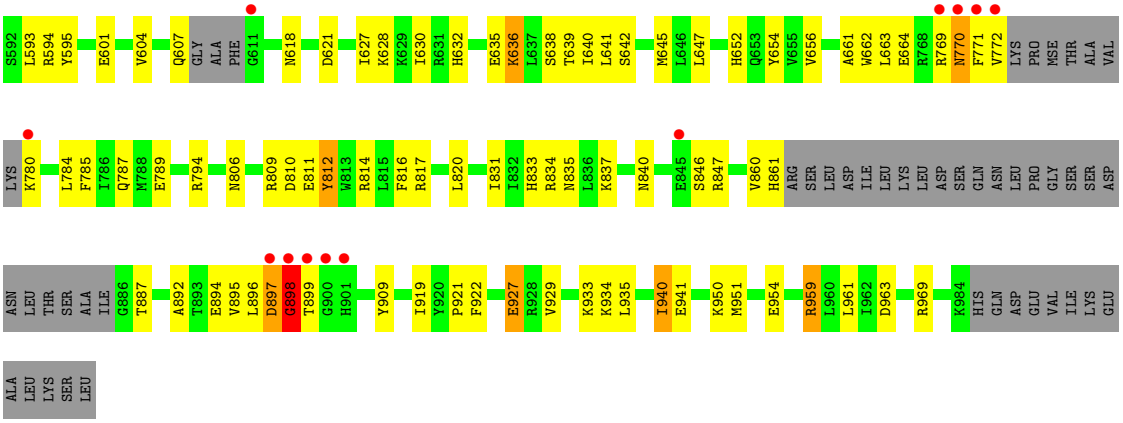
• Molecule 1: Serine/threonine-protein kinase

Chain C:



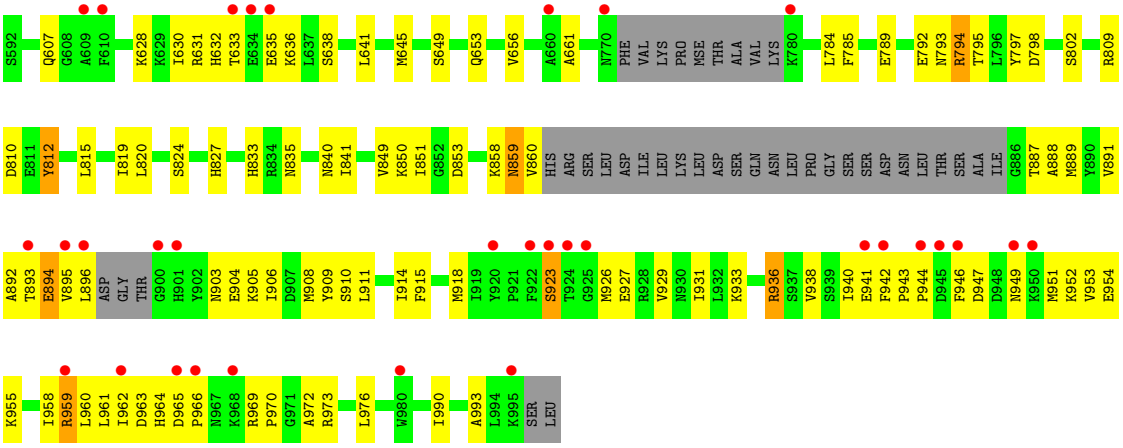
• Molecule 1: Serine/threonine-protein kinase

Chain D:



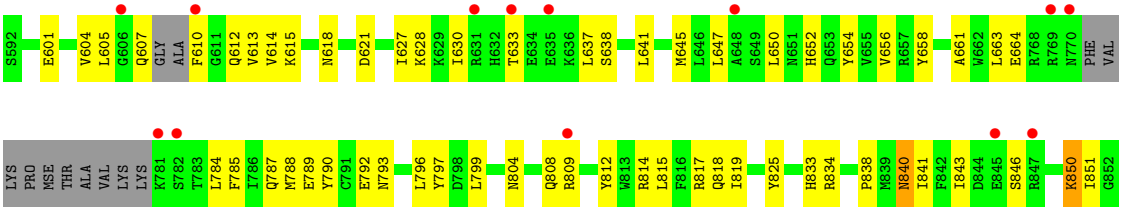
• Molecule 1: Serine/threonine-protein kinase

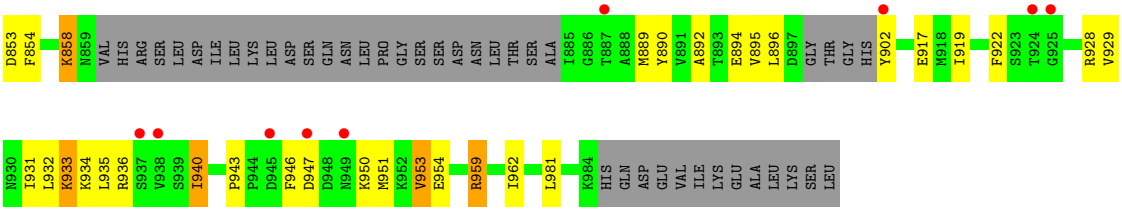
Chain E:



• Molecule 1: Serine/threonine-protein kinase

Chain F:




D853
F854
K858
N859
VAL
HIS
ARG
SER
LEU
ASP
ILE
LEU
LYS
LEU
ASP
SER
GLN
ASN
LEU
PRO
GLY
SER
SER
ASP
ASN
LEU
THR
SER
ALA
I885
G886
T887
A888
M889
Y890
V891
A892
T893
E894
V895
L896
D897
GLY
THR
GLY
HIS
Y902
E917
M918
I919
F922
S923
T924
G925
R928
V929
N930
I931
L932
K933
K934
L935
R936
S937
V938
S939
I940
P943
P944
D945
F946
D947
D948
N949
K950
M951
K952
V953
E954
R959
I962
L981
K984
HIS
GLN
ASP
GLU
VAL
ILE
LYS
GLU
ALA
LEU
LYS
SER
LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	79.56Å 154.14Å 157.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.35 – 2.60 35.35 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.6 (35.35-2.60) 96.8 (35.35-2.35)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.74 (at 2.34Å)	Xtriage
Refinement program	CNX 2000.1	Depositor
R, R_{free}	0.204 , 0.252 0.210 , 0.254	Depositor DCC
R_{free} test set	1590 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å^2)	49.3	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 53.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13242	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.29% 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

5.1 Standard geometry

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

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	0.57	0/2257	0.72	1/3021 (0.0%)
1	B	0.63	0/2114	0.75	0/2831
1	C	0.56	0/2295	0.71	1/3075 (0.0%)
1	D	0.55	0/2151	0.73	1/2881 (0.0%)
1	E	0.46	0/2215	0.61	0/2965
1	F	0.45	0/2098	0.58	0/2808
All	All	0.54	0/13130	0.69	3/17581 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	884	ALA	N-CA-C	-8.81	87.21	111.00
1	D	898	GLY	N-CA-C	6.53	129.43	113.10
1	A	657	ARG	NE-CZ-NH2	-5.31	117.64	120.30

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	2222	0	2246	72	0
1	B	2081	0	2098	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2259	0	2283	55	0
1	D	2117	0	2133	65	0
1	E	2181	0	2204	85	0
1	F	2067	0	2085	81	0
2	A	6	0	4	0	0
2	B	6	0	4	0	0
2	C	6	0	4	0	0
2	D	6	0	4	0	0
2	E	6	0	4	0	0
2	F	6	0	4	0	0
3	A	67	0	0	5	0
3	B	51	0	0	5	0
3	C	57	0	0	2	0
3	D	72	0	0	5	0
3	E	11	0	0	0	0
3	F	21	0	0	1	0
All	All	13242	0	13073	383	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 15.

The worst 5 of 383 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:652:HIS:HD2	1:C:654:TYR:H	1.10	0.95
1:F:601:GLU:HG3	1:F:614:VAL:HG11	1.48	0.93
1:A:784:LEU:HD11	1:B:645:MSE:HE2	1.53	0.89
1:B:837:LYS:HD2	1:B:887:THR:HG21	1.57	0.87
1:E:915:PHE:HA	1:E:918:MSE:HE3	1.56	0.86

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	261/303 (86%)	248 (95%)	11 (4%)	2 (1%)	19 39
1	B	244/303 (80%)	230 (94%)	13 (5%)	1 (0%)	34 57
1	C	269/303 (89%)	251 (93%)	15 (6%)	3 (1%)	14 30
1	D	248/303 (82%)	236 (95%)	8 (3%)	4 (2%)	9 19
1	E	256/303 (84%)	232 (91%)	22 (9%)	2 (1%)	19 39
1	F	239/303 (79%)	214 (90%)	21 (9%)	4 (2%)	9 18
All	All	1517/1818 (83%)	1411 (93%)	90 (6%)	16 (1%)	14 30

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	898	GLY
1	B	609	ALA
1	D	770	ASN
1	E	894	GLU
1	F	896	LEU

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	241/263 (92%)	236 (98%)	5 (2%)	53 77
1	B	226/263 (86%)	221 (98%)	5 (2%)	52 76
1	C	246/263 (94%)	240 (98%)	6 (2%)	49 74
1	D	231/263 (88%)	223 (96%)	8 (4%)	36 62
1	E	237/263 (90%)	222 (94%)	15 (6%)	18 36
1	F	226/263 (86%)	215 (95%)	11 (5%)	25 48
All	All	1407/1578 (89%)	1357 (96%)	50 (4%)	35 61

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	858	LYS
1	E	947	ASP
1	F	981	LEU
1	E	859	ASN
1	E	936	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	653	GLN
1	F	804	ASN
1	F	840	ASN
1	C	652	HIS
1	C	612	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

6 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	$\#\|Z\|>2$
2	GOL	E	998	-	5,5,5	4.33	5 (100%)	5,5,5	5.68	3 (60%)
2	GOL	D	698	-	5,5,5	4.52	5 (100%)	5,5,5	5.70	3 (60%)
2	GOL	B	498	-	5,5,5	4.58	5 (100%)	5,5,5	5.65	3 (60%)
2	GOL	F	998	-	5,5,5	4.51	5 (100%)	5,5,5	5.47	3 (60%)
2	GOL	A	398	-	5,5,5	4.66	5 (100%)	5,5,5	5.66	3 (60%)
2	GOL	C	998	-	5,5,5	4.60	5 (100%)	5,5,5	5.70	3 (60%)

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
2	GOL	E	998	-	-	2/4/4/4	-
2	GOL	D	698	-	-	3/4/4/4	-
2	GOL	B	498	-	-	2/4/4/4	-
2	GOL	F	998	-	-	2/4/4/4	-
2	GOL	A	398	-	-	3/4/4/4	-
2	GOL	C	998	-	-	3/4/4/4	-

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	998	GOL	C3-C2	-7.58	1.20	1.51
2	A	398	GOL	C3-C2	-7.48	1.21	1.51
2	D	698	GOL	C3-C2	-7.42	1.21	1.51
2	B	498	GOL	C3-C2	-7.41	1.21	1.51
2	F	998	GOL	C3-C2	-7.20	1.22	1.51

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	698	GOL	O3-C3-C2	10.26	159.38	110.20
2	C	998	GOL	O3-C3-C2	10.22	159.21	110.20
2	E	998	GOL	O3-C3-C2	10.15	158.87	110.20
2	B	498	GOL	O3-C3-C2	10.03	158.27	110.20
2	A	398	GOL	O3-C3-C2	9.95	157.90	110.20

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	398	GOL	C1-C2-C3-O3
2	B	498	GOL	C1-C2-C3-O3
2	C	998	GOL	C1-C2-C3-O3
2	D	698	GOL	C1-C2-C3-O3
2	E	998	GOL	O1-C1-C2-O2

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 (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^{th} 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	261/303 (86%)	-0.09	4 (1%) 73 70	25, 43, 73, 94	0
1	B	244/303 (80%)	-0.01	16 (6%) 18 13	21, 38, 72, 94	0
1	C	267/303 (88%)	0.05	13 (4%) 29 23	25, 44, 81, 96	0
1	D	248/303 (81%)	-0.04	12 (4%) 30 24	28, 44, 77, 92	0
1	E	256/303 (84%)	0.58	32 (12%) 3 2	36, 69, 97, 100	0
1	F	241/303 (79%)	0.41	22 (9%) 9 6	40, 69, 91, 102	0
All	All	1517/1818 (83%)	0.15	99 (6%) 18 14	21, 50, 89, 102	0

The worst 5 of 99 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	882	THR	5.9
1	D	899	THR	5.8
1	B	769	ARG	5.7
1	D	772	VAL	5.7
1	E	949	ASN	5.6

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 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, 95^{th} 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(Å^2)	Q<0.9
2	GOL	F	998	6/6	0.70	0.32	77,81,82,82	0
2	GOL	E	998	6/6	0.87	0.19	48,57,60,62	0
2	GOL	D	698	6/6	0.88	0.26	46,56,58,65	0
2	GOL	C	998	6/6	0.94	0.20	37,47,49,52	0
2	GOL	A	398	6/6	0.95	0.18	33,46,50,61	0
2	GOL	B	498	6/6	0.96	0.21	40,47,50,57	0

6.5 Other polymers

There are no such residues in this entry.