



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 09:00 pm GMT

PDB ID : 4DIP
Title : Crystal structure of human Peptidyl-prolyl cis-trans isomerase FKBP14
Authors : Krojer, T.; Kiyani, W.; Goubin, S.; Muniz, J.R.C.; Filippakopoulos, P.; Arrowsmith, C.H.; Edwards, A.; Bountra, C.; von Delft, F.; Oppermann, U.; Zschocke, J.; Yue, W.W.; Structural Genomics Consortium (SGC)
Deposited on : 2012-01-31
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

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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

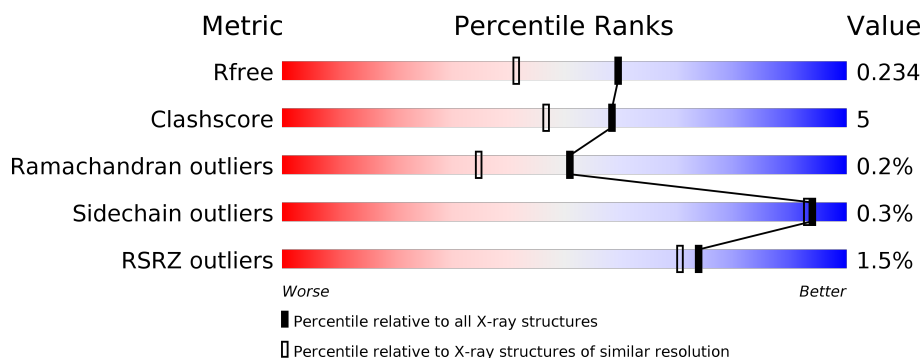
1 Overall quality at a glance

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}	100719	5868 (1.84-1.80)
Clashscore	112137	6856 (1.84-1.80)
Ramachandran outliers	110173	6780 (1.84-1.80)
Sidechain outliers	110143	6780 (1.84-1.80)
RSRZ outliers	101464	5947 (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 ≥ 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	125	
1	B	125	
1	C	125	
1	D	125	
1	E	125	
1	F	125	

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Mol	Chain	Length	Quality of chain
1	G	125	<div><div></div><div>2%</div><div>90%</div><div>6%</div><div></div><div></div></div>
1	H	125	<div><div></div><div>2%</div><div>87%</div><div>8%</div><div>5%</div><div></div></div>
1	I	125	<div><div></div><div>3%</div><div>84%</div><div>13%</div><div></div><div></div></div>
1	J	125	<div><div></div><div>3%</div><div>86%</div><div>8%</div><div>5%</div><div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10301 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 Peptidyl-prolyl cis-trans isomerase FKBP14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	121	Total	C	N	O	S	0	4	0
			967	628	162	171	6			
1	B	121	Total	C	N	O	S	0	3	0
			954	620	158	170	6			
1	C	120	Total	C	N	O	S	0	2	0
			948	619	160	165	4			
1	D	120	Total	C	N	O	S	0	2	0
			942	613	159	165	5			
1	E	120	Total	C	N	O	S	0	3	0
			946	616	159	166	5			
1	F	120	Total	C	N	O	S	0	3	0
			945	617	158	166	4			
1	G	120	Total	C	N	O	S	0	3	0
			950	620	162	164	4			
1	H	119	Total	C	N	O	S	0	0	0
			930	603	159	164	4			
1	I	121	Total	C	N	O	S	0	1	0
			940	610	157	167	6			
1	J	119	Total	C	N	O	S	0	2	0
			920	597	156	162	5			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	TYR	-	EXPRESSION TAG	UNP Q9NWM8
A	15	PHE	-	EXPRESSION TAG	UNP Q9NWM8
A	16	GLN	-	EXPRESSION TAG	UNP Q9NWM8
A	17	SER	-	EXPRESSION TAG	UNP Q9NWM8
A	18	MET	-	EXPRESSION TAG	UNP Q9NWM8
B	14	TYR	-	EXPRESSION TAG	UNP Q9NWM8
B	15	PHE	-	EXPRESSION TAG	UNP Q9NWM8
B	16	GLN	-	EXPRESSION TAG	UNP Q9NWM8
B	17	SER	-	EXPRESSION TAG	UNP Q9NWM8

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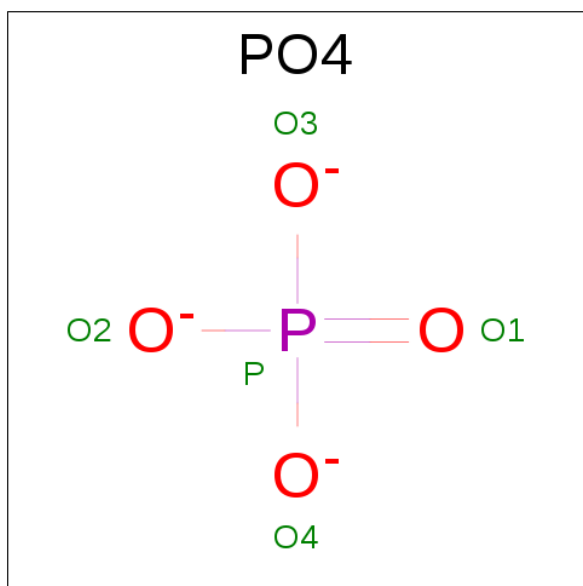
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Chain	Residue	Modelled	Actual	Comment	Reference
B	18	MET	-	EXPRESSION TAG	UNP Q9NWM8
C	14	TYR	-	EXPRESSION TAG	UNP Q9NWM8
C	15	PHE	-	EXPRESSION TAG	UNP Q9NWM8
C	16	GLN	-	EXPRESSION TAG	UNP Q9NWM8
C	17	SER	-	EXPRESSION TAG	UNP Q9NWM8
C	18	MET	-	EXPRESSION TAG	UNP Q9NWM8
D	14	TYR	-	EXPRESSION TAG	UNP Q9NWM8
D	15	PHE	-	EXPRESSION TAG	UNP Q9NWM8
D	16	GLN	-	EXPRESSION TAG	UNP Q9NWM8
D	17	SER	-	EXPRESSION TAG	UNP Q9NWM8
D	18	MET	-	EXPRESSION TAG	UNP Q9NWM8
E	14	TYR	-	EXPRESSION TAG	UNP Q9NWM8
E	15	PHE	-	EXPRESSION TAG	UNP Q9NWM8
E	16	GLN	-	EXPRESSION TAG	UNP Q9NWM8
E	17	SER	-	EXPRESSION TAG	UNP Q9NWM8
E	18	MET	-	EXPRESSION TAG	UNP Q9NWM8
F	14	TYR	-	EXPRESSION TAG	UNP Q9NWM8
F	15	PHE	-	EXPRESSION TAG	UNP Q9NWM8
F	16	GLN	-	EXPRESSION TAG	UNP Q9NWM8
F	17	SER	-	EXPRESSION TAG	UNP Q9NWM8
F	18	MET	-	EXPRESSION TAG	UNP Q9NWM8
G	14	TYR	-	EXPRESSION TAG	UNP Q9NWM8
G	15	PHE	-	EXPRESSION TAG	UNP Q9NWM8
G	16	GLN	-	EXPRESSION TAG	UNP Q9NWM8
G	17	SER	-	EXPRESSION TAG	UNP Q9NWM8
G	18	MET	-	EXPRESSION TAG	UNP Q9NWM8
H	14	TYR	-	EXPRESSION TAG	UNP Q9NWM8
H	15	PHE	-	EXPRESSION TAG	UNP Q9NWM8
H	16	GLN	-	EXPRESSION TAG	UNP Q9NWM8
H	17	SER	-	EXPRESSION TAG	UNP Q9NWM8
H	18	MET	-	EXPRESSION TAG	UNP Q9NWM8
I	14	TYR	-	EXPRESSION TAG	UNP Q9NWM8
I	15	PHE	-	EXPRESSION TAG	UNP Q9NWM8
I	16	GLN	-	EXPRESSION TAG	UNP Q9NWM8
I	17	SER	-	EXPRESSION TAG	UNP Q9NWM8
I	18	MET	-	EXPRESSION TAG	UNP Q9NWM8
J	14	TYR	-	EXPRESSION TAG	UNP Q9NWM8
J	15	PHE	-	EXPRESSION TAG	UNP Q9NWM8
J	16	GLN	-	EXPRESSION TAG	UNP Q9NWM8
J	17	SER	-	EXPRESSION TAG	UNP Q9NWM8
J	18	MET	-	EXPRESSION TAG	UNP Q9NWM8

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Na	0	0
			1	1		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	G	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	72	Total	O	0	0
			72	72		
4	B	90	Total	O	0	0
			90	90		
4	C	84	Total	O	0	0
			84	84		
4	D	105	Total	O	0	0
			105	105		
4	E	90	Total	O	0	0
			90	90		
4	F	91	Total	O	0	0
			91	91		
4	G	102	Total	O	0	0
			102	102		
4	H	86	Total	O	0	0
			86	86		

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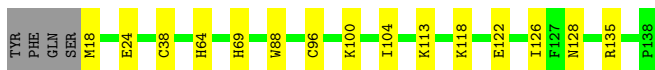
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	70	Total 70	O 70	0	0
4	J	63	Total 63	O 63	0	0

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 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: Peptidyl-prolyl cis-trans isomerase FKBP14

Chain A: 




- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP14

Chain B: 




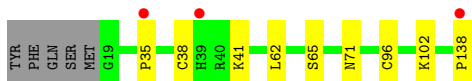
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP14

Chain C: 




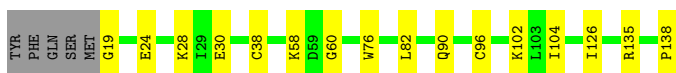
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP14

Chain D: 




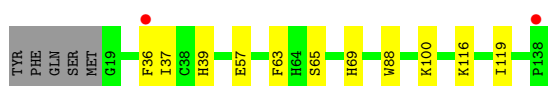
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP14

Chain E: 

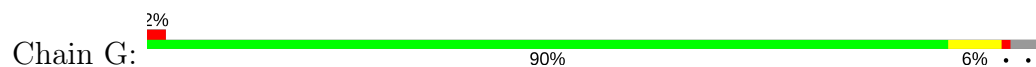


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP14

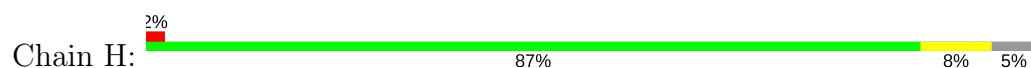
Chain F: 



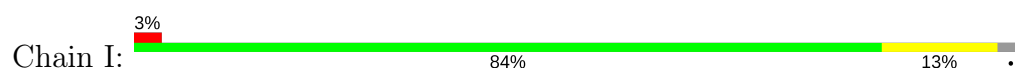
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP14



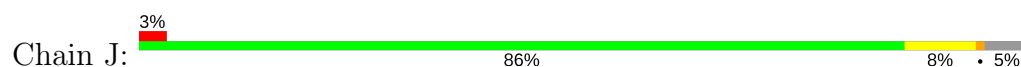
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP14



- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP14



- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP14



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	63.12Å 64.06Å 80.81Å 81.23° 75.21° 73.38°	Depositor
Resolution (Å)	58.95 – 1.82 53.05 – 1.82	Depositor EDS
% Data completeness (in resolution range)	96.6 (58.95-1.82) 93.8 (53.05-1.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 1.82Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.203 , 0.231 0.206 , 0.234	Depositor DCC
R_{free} test set	5064 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	15.7	Xtrriage
Anisotropy	0.242	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 51.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.36$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10301	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.28 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.8051e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, PO4

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	0.75	1/1000 (0.1%)	0.83	1/1348 (0.1%)
1	B	0.77	1/987 (0.1%)	0.82	0/1332
1	C	0.79	0/979	0.84	1/1320 (0.1%)
1	D	0.77	0/972	0.82	1/1311 (0.1%)
1	E	0.80	1/979 (0.1%)	0.84	2/1323 (0.2%)
1	F	0.78	1/979 (0.1%)	0.83	0/1322
1	G	0.76	0/983	0.87	3/1325 (0.2%)
1	H	0.73	1/953 (0.1%)	0.80	0/1284
1	I	0.68	0/966	0.80	0/1303
1	J	0.70	1/947 (0.1%)	0.81	0/1278
All	All	0.75	6/9745 (0.1%)	0.82	8/13146 (0.1%)

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	B	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	76	TRP	CD2-CE2	6.28	1.48	1.41
1	A	88	TRP	CD2-CE2	6.06	1.48	1.41
1	J	53	GLU	CD-OE2	-5.52	1.19	1.25
1	H	76	TRP	CD2-CE2	5.33	1.47	1.41
1	E	76	TRP	CD2-CE2	5.26	1.47	1.41
1	F	88	TRP	CD2-CE2	5.18	1.47	1.41

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	38	CYS	CA-CB-SG	7.18	126.93	114.00
1	D	102	LYS	CD-CE-NZ	5.60	124.58	111.70
1	A	135	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	G	116	LYS	CB-CG-CD	5.20	125.13	111.60
1	E	135	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	G	116	LYS	CD-CE-NZ	-5.15	99.86	111.70
1	C	56	LEU	CB-CG-CD1	-5.07	102.39	111.00
1	E	90	GLN	CA-CB-CG	-5.04	102.32	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	137	GLY	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	967	0	986	12	1
1	B	954	0	960	15	0
1	C	948	0	968	5	0
1	D	942	0	959	9	0
1	E	946	0	963	17	0
1	F	945	0	962	8	0
1	G	950	0	983	9	0
1	H	930	0	948	6	0
1	I	940	0	941	17	0
1	J	920	0	939	8	0
2	B	1	0	0	0	0
3	G	5	0	0	0	0
4	A	72	0	0	7	1
4	B	90	0	0	8	0
4	C	84	0	0	3	0
4	D	105	0	0	5	0
4	E	90	0	0	8	0
4	F	91	0	0	1	0
4	G	102	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	86	0	0	1	1
4	I	70	0	0	4	0
4	J	63	0	0	1	1
All	All	10301	0	9609	104	2

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 5.

All (104) 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:96[B]:CYS:SG	4:B:337:HOH:O	2.12	1.04
1:B:133[A]:GLU:OE1	4:B:386:HOH:O	1.74	1.03
4:B:389:HOH:O	1:F:36:PHE:CZ	2.18	0.94
1:C:86:LYS:HE2	4:C:264:HOH:O	1.68	0.93
1:J:38:CYS:SG	1:J:96[B]:CYS:HB3	2.12	0.90
1:I:56:LEU:HD21	1:I:119:ILE:HD13	1.56	0.87
4:B:389:HOH:O	1:F:36:PHE:HZ	1.53	0.86
1:B:57:GLU:HG2	4:B:388:HOH:O	1.80	0.82
1:G:126:ILE:HG22	4:G:380:HOH:O	1.82	0.78
1:D:38:CYS:SG	1:D:96[B]:CYS:HB3	2.25	0.77
1:B:64:HIS:HD2	4:B:381:HOH:O	1.65	0.77
1:A:64:HIS:HD2	4:A:267:HOH:O	1.66	0.76
1:A:38:CYS:SG	1:A:96[B]:CYS:HB3	2.25	0.76
1:E:82:LEU:O	1:E:82:LEU:CD2	2.33	0.76
1:I:63:PHE:CD2	1:I:119:ILE:HD11	2.21	0.75
1:H:33:GLN:HG3	1:H:100:LYS:HD3	1.66	0.75
1:I:38:CYS:SG	1:I:96[B]:CYS:HB3	2.27	0.75
1:I:63:PHE:CG	1:I:119:ILE:HD11	2.22	0.75
1:I:104:ILE:HG12	4:I:248:HOH:O	1.87	0.74
1:E:38:CYS:SG	1:E:96[B]:CYS:HB3	2.28	0.72
1:H:34:LYS:HE3	1:H:38:CYS:SG	2.33	0.69
1:A:18:MET:N	4:A:266:HOH:O	2.27	0.67
4:A:230:HOH:O	1:H:130:ASP:HB3	1.95	0.66
1:I:118:LYS:NZ	4:I:264:HOH:O	2.01	0.66
1:E:82:LEU:HD23	1:E:82:LEU:O	1.96	0.66
1:I:56:LEU:HD21	1:I:119:ILE:CD1	2.25	0.65
1:B:38:CYS:SG	1:B:96[B]:CYS:HB3	2.36	0.65
1:A:113:LYS:CD	1:A:122:GLU:OE2	2.45	0.65
1:A:24[A]:GLU:HB2	4:A:268:HOH:O	1.95	0.65
1:B:133[A]:GLU:OE2	1:F:100:LYS:NZ	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:30:GLU:OE1	1:E:102:LYS:HE2	1.98	0.64
1:A:24[B]:GLU:HB2	4:A:268:HOH:O	1.96	0.64
1:E:138:PRO:C	4:E:289:HOH:O	2.38	0.62
1:E:104:ILE:HG12	1:E:126:ILE:HD12	1.80	0.61
1:G:38:CYS:SG	4:G:395:HOH:O	2.56	0.61
1:D:138:PRO:HD2	4:D:262:HOH:O	2.00	0.61
1:I:58:LYS:HB3	4:I:243:HOH:O	2.01	0.61
1:E:82:LEU:HD22	1:E:82:LEU:O	2.01	0.60
1:J:111:TYR:CE2	1:J:119:ILE:HD13	2.36	0.60
1:G:34:LYS:HE3	1:G:38:CYS:SG	2.43	0.59
1:E:28:LYS:HD3	1:E:104:ILE:HD12	1.86	0.58
1:E:19:GLY:N	4:E:224:HOH:O	2.37	0.57
1:F:65:SER:H	1:F:69:HIS:HD1	1.52	0.57
1:E:82:LEU:HD23	1:E:82:LEU:C	2.24	0.56
1:E:60:GLY:HA2	4:E:279:HOH:O	2.06	0.56
1:H:73:GLN:HG3	4:H:285:HOH:O	2.05	0.56
1:E:82:LEU:CD2	4:E:219:HOH:O	2.55	0.55
1:A:64:HIS:CD2	4:A:267:HOH:O	2.48	0.55
1:C:138:PRO:HD2	4:C:282:HOH:O	2.06	0.55
1:G:38:CYS:CB	4:G:395:HOH:O	2.55	0.55
1:B:122:GLU:OE2	1:B:122:GLU:HA	2.07	0.54
1:I:38:CYS:SG	1:I:96[B]:CYS:CB	2.92	0.53
1:B:132:LEU:O	1:B:133[B]:GLU:HG2	2.10	0.52
1:B:113:LYS:NZ	4:B:311:HOH:O	2.23	0.51
1:D:138:PRO:N	4:D:221:HOH:O	2.44	0.51
1:G:38:CYS:C	4:G:395:HOH:O	2.49	0.50
1:C:111:TYR:CE2	1:C:119:ILE:HD13	2.46	0.50
1:I:32:LEU:HD12	1:I:100:LYS:HG2	1.94	0.50
1:D:35:PRO:HD2	1:D:96[B]:CYS:SG	2.52	0.50
1:G:127:PHE:C	4:G:380:HOH:O	2.50	0.49
1:A:69:HIS:NE2	1:A:118:LYS:NZ	2.61	0.48
1:D:62:LEU:HD11	1:D:65:SER:HB3	1.95	0.48
1:B:113:LYS:CE	4:B:311:HOH:O	2.61	0.47
1:C:70:ASN:HA	4:C:242:HOH:O	2.14	0.47
1:G:33:GLN:HG2	4:G:343:HOH:O	2.14	0.47
1:D:41:LYS:HD3	4:D:300:HOH:O	2.15	0.47
1:E:58:LYS:CG	4:E:204:HOH:O	2.62	0.46
1:B:132:LEU:O	1:B:133[B]:GLU:CG	2.63	0.46
1:F:63:PHE:CD1	1:F:119:ILE:HD11	2.50	0.46
1:A:100:LYS:HE3	1:A:128:ASN:HB3	1.98	0.46
1:I:104:ILE:HD12	1:I:126:ILE:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:42:THR:HG21	1:J:48:MET:CE	2.46	0.45
1:A:69:HIS:HE2	1:A:118:LYS:NZ	2.14	0.45
1:C:100:LYS:HE3	4:E:223:HOH:O	2.17	0.45
1:F:116:LYS:HB2	1:F:119:ILE:HB	1.99	0.45
1:B:32:LEU:HD12	1:B:100:LYS:HG2	1.99	0.45
1:B:122:GLU:OE2	1:B:122:GLU:CA	2.66	0.44
1:G:37:ILE:HG23	1:G:39:HIS:CE1	2.53	0.44
1:I:21:LEU:CD1	4:I:269:HOH:O	2.65	0.44
1:J:42:THR:HG21	1:J:48:MET:HE3	2.00	0.44
1:A:38:CYS:SG	1:A:96[B]:CYS:CB	2.99	0.44
1:F:37:ILE:HG23	1:F:39[A]:HIS:CE1	2.52	0.43
1:A:104:ILE:HD12	1:A:126:ILE:HG12	2.00	0.43
1:E:38:CYS:SG	1:E:96[B]:CYS:CB	3.00	0.43
1:F:57:GLU:OE2	4:F:377:HOH:O	2.21	0.43
1:D:138:PRO:CD	4:D:221:HOH:O	2.67	0.43
1:B:100:LYS:HG3	1:B:130:ASP:OD1	2.18	0.42
1:D:38:CYS:SG	1:D:96[B]:CYS:CB	2.98	0.42
1:I:100:LYS:HG3	1:I:130:ASP:OD1	2.20	0.42
1:E:82:LEU:HD21	4:E:275:HOH:O	2.18	0.42
1:I:42:THR:HG21	1:I:48:MET:CE	2.50	0.42
1:I:17:SER:HB3	1:J:83:GLU:HG2	2.01	0.42
1:J:135:ARG:HD3	4:J:232:HOH:O	2.19	0.42
1:J:111:TYR:CD2	1:J:119:ILE:HD13	2.54	0.42
1:G:38:CYS:HB2	4:G:363:HOH:O	2.19	0.42
1:H:28:LYS:HD3	1:H:104:ILE:HD12	2.02	0.41
1:E:82:LEU:CD2	1:E:82:LEU:C	2.85	0.41
1:E:24:GLU:OE2	4:E:232:HOH:O	2.21	0.41
4:A:220:HOH:O	1:H:36:PHE:HD2	2.04	0.41
1:D:138:PRO:HD3	4:D:221:HOH:O	2.21	0.41
1:I:104:ILE:CD1	1:I:126:ILE:HG12	2.51	0.41
1:I:63:PHE:CD2	1:I:119:ILE:CD1	2.99	0.41
1:B:62:LEU:HD11	1:B:65:SER:HB3	2.03	0.40
1:J:63:PHE:CB	1:J:118:LYS:HD2	2.52	0.40

All (2) 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:24[B]:GLU:OE2	4:H:239:HOH:O[1_455]	2.05	0.15
4:A:224:HOH:O	4:J:259:HOH:O[1_545]	2.18	0.02

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	123/125 (98%)	119 (97%)	4 (3%)	0	100	100
1	B	122/125 (98%)	120 (98%)	1 (1%)	1 (1%)	22	8
1	C	120/125 (96%)	116 (97%)	3 (2%)	1 (1%)	22	8
1	D	120/125 (96%)	119 (99%)	1 (1%)	0	100	100
1	E	121/125 (97%)	120 (99%)	1 (1%)	0	100	100
1	F	121/125 (97%)	116 (96%)	5 (4%)	0	100	100
1	G	121/125 (97%)	118 (98%)	3 (2%)	0	100	100
1	H	117/125 (94%)	114 (97%)	3 (3%)	0	100	100
1	I	120/125 (96%)	118 (98%)	2 (2%)	0	100	100
1	J	119/125 (95%)	116 (98%)	3 (2%)	0	100	100
All	All	1204/1250 (96%)	1176 (98%)	26 (2%)	2 (0%)	51	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	19	GLY
1	C	117	GLY

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	104/106 (98%)	104 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	101/106 (95%)	101 (100%)	0	100	100
1	C	101/106 (95%)	101 (100%)	0	100	100
1	D	100/106 (94%)	99 (99%)	1 (1%)	80	74
1	E	101/106 (95%)	101 (100%)	0	100	100
1	F	101/106 (95%)	101 (100%)	0	100	100
1	G	102/106 (96%)	101 (99%)	1 (1%)	80	74
1	H	99/106 (93%)	99 (100%)	0	100	100
1	I	98/106 (92%)	98 (100%)	0	100	100
1	J	97/106 (92%)	96 (99%)	1 (1%)	80	74
All	All	1004/1060 (95%)	1001 (100%)	3 (0%)	94	93

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

Mol	Chain	Res	Type
1	D	71	ASN
1	G	38	CYS
1	J	118	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	128	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 [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	PO4	G	201	-	4,4,4	0.65	0	6,6,6	1.27	1 (16%)

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	PO4	G	201	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	201	PO4	O4-P-O2	2.03	115.35	107.90

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 [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	121/125 (96%)	-0.07	0 100 100	9, 20, 41, 59	0
1	B	121/125 (96%)	-0.20	0 100 100	9, 18, 38, 54	0
1	C	120/125 (96%)	-0.13	1 (0%) 86 84	8, 17, 37, 53	0
1	D	120/125 (96%)	-0.17	3 (2%) 58 53	9, 16, 30, 43	1 (0%)
1	E	120/125 (96%)	-0.30	0 100 100	9, 16, 28, 39	0
1	F	120/125 (96%)	-0.21	2 (1%) 70 67	9, 18, 30, 67	0
1	G	120/125 (96%)	-0.28	2 (1%) 70 67	9, 15, 27, 50	0
1	H	119/125 (95%)	-0.18	2 (1%) 70 67	10, 19, 31, 36	0
1	I	121/125 (96%)	0.01	4 (3%) 47 41	10, 21, 47, 60	0
1	J	119/125 (95%)	-0.08	4 (3%) 46 40	10, 20, 48, 80	0
All	All	1201/1250 (96%)	-0.16	18 (1%) 74 70	8, 18, 37, 80	1 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	38	CYS	5.4
1	C	36[A]	PHE	4.1
1	J	37	ILE	4.0
1	F	138	PRO	3.6
1	D	138	PRO	3.5
1	I	39	HIS	3.4
1	J	39	HIS	3.0
1	G	138	PRO	3.0
1	I	38	CYS	2.9
1	F	36	PHE	2.8
1	I	119	ILE	2.6
1	I	136	ASN	2.5
1	H	39	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	35	PRO	2.4
1	D	39	HIS	2.4
1	H	36	PHE	2.3
1	J	67	HIS	2.3
1	G	39	HIS	2.1

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	PO4	G	201	5/5	0.97	0.12	0.26	24,25,30,44	0
2	NA	B	201	1/1	0.96	0.22	-	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.