wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 07:04 PM GMT

PDB ID	:	1DU3
Title	:	Crystal structure of TRAIL-SDR5
Authors	:	Cha, S.-S.; Sung, B.-J.; Oh, B.-H.
Deposited on	:	2000-01-14
Resolution	:	2.20 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

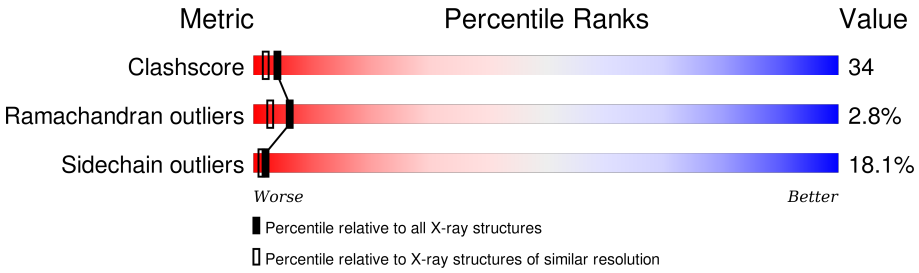
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 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))
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)

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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	130	25% 36% 8% 31%
1	B	130	34% 39% 12% 15%
1	C	130	18% 38% 12% • 31%
1	G	130	33% 40% 10% 17%
1	H	130	28% 31% 10% • 31%
1	I	130	22% 34% 12% • 31%
2	D	168	46% 38% 5% • 10%

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Mol	Chain	Length	Quality of chain
2	E	168	40% 39% 9% 10%
2	F	168	36% 48% 7% 10%
2	J	168	46% 39% 10%
2	K	168	43% 39% 5% 10%
2	L	168	36% 45% 10% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ZN	E	1	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12108 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 DEATH RECEPTOR 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	90	Total	C	N	O	S	0	0	0
			701	419	122	148	12			
1	B	110	Total	C	N	O	S	0	0	0
			833	497	148	172	16			
1	C	90	Total	C	N	O	S	0	0	0
			697	417	121	147	12			
1	G	108	Total	C	N	O	S	0	0	0
			833	498	150	169	16			
1	H	90	Total	C	N	O	S	0	0	0
			691	414	118	147	12			
1	I	90	Total	C	N	O	S	0	0	0
			701	419	122	148	12			

- Molecule 2 is a protein called TNF-RELATED APOPTOSIS INDUCING LIGAND.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	152	Total	C	N	O	S	0	0	0
			1252	797	217	234	4			
2	E	152	Total	C	N	O	S	0	0	0
			1252	797	217	234	4			
2	F	152	Total	C	N	O	S	0	0	0
			1246	794	214	234	4			
2	J	152	Total	C	N	O	S	0	0	0
			1248	795	217	232	4			
2	K	152	Total	C	N	O	S	0	0	0
			1252	797	217	234	4			
2	L	152	Total	C	N	O	S	0	0	0
			1238	789	212	233	4			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	K	1	Total Zn 1 1	0	0
3	E	1	Total Zn 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	26	Total O 26 26	0	0
4	B	23	Total O 23 23	0	0
4	C	6	Total O 6 6	0	0
4	D	22	Total O 22 22	0	0
4	E	14	Total O 14 14	0	0
4	F	13	Total O 13 13	0	0
4	G	16	Total O 16 16	0	0
4	H	7	Total O 7 7	0	0
4	I	11	Total O 11 11	0	0
4	J	8	Total O 8 8	0	0
4	K	9	Total O 9 9	0	0
4	L	7	Total O 7 7	0	0

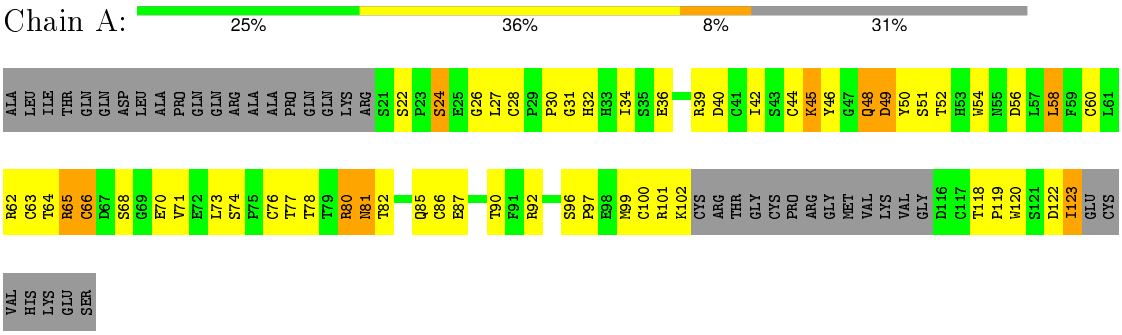
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

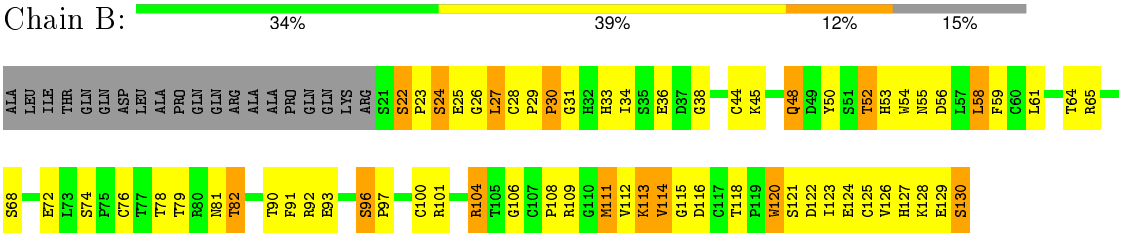
- Molecule 1: DEATH RECEPTOR 5

Chain A:



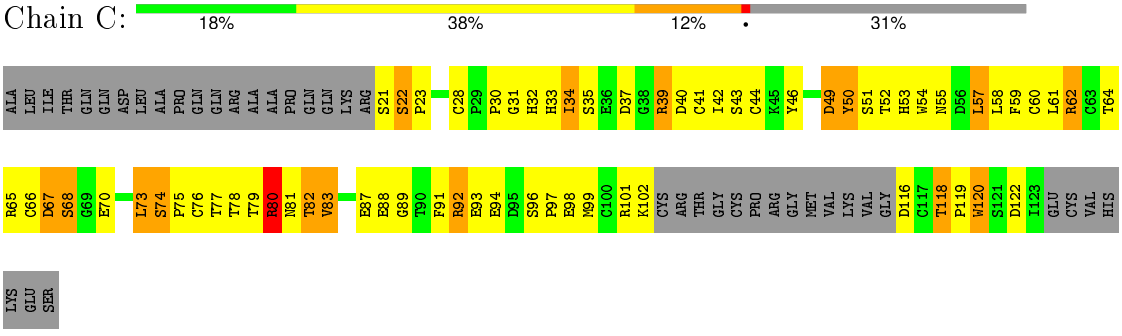
- Molecule 1: DEATH RECEPTOR 5

Chain B:



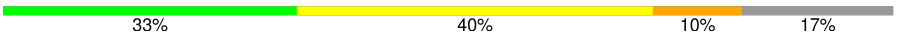
- Molecule 1: DEATH RECEPTOR 5

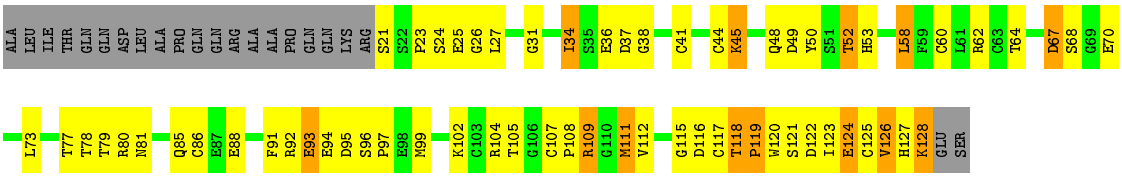
Chain C:



- Molecule 1: DEATH RECEPTOR 5

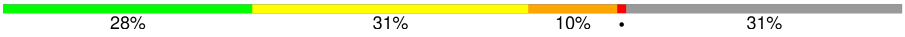
Chain G:

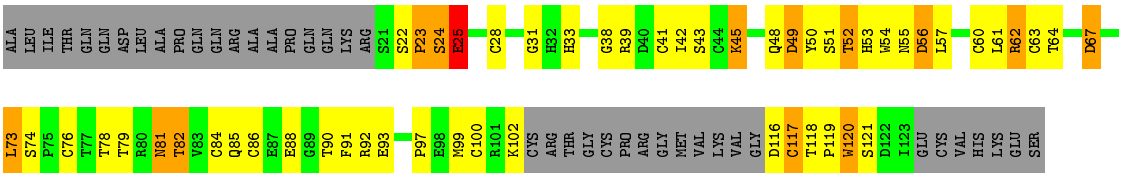




- Molecule 1: DEATH RECEPTOR 5

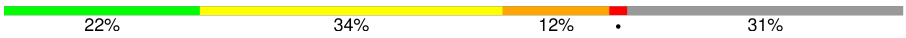
Chain H:

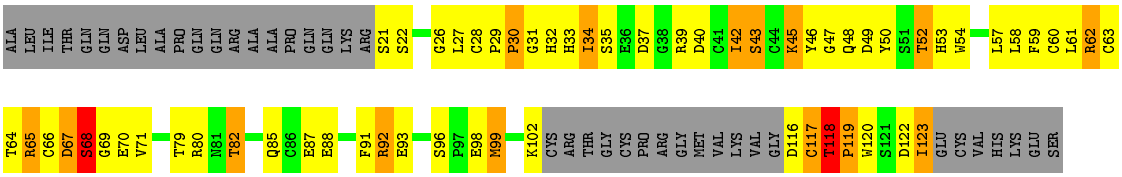




- Molecule 1: DEATH RECEPTOR 5

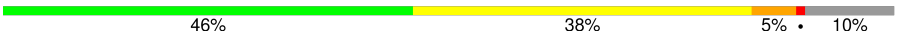
Chain I:

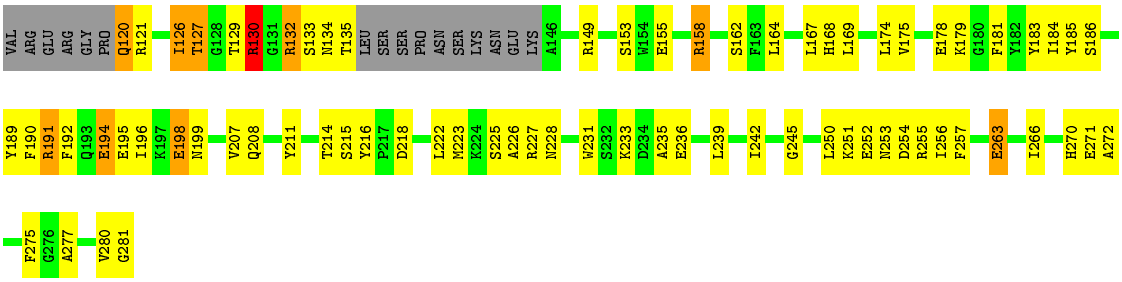




- Molecule 2: TNF-RELATED APOPTOSIS INDUCING LIGAND

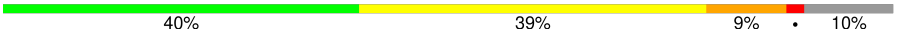
Chain D:

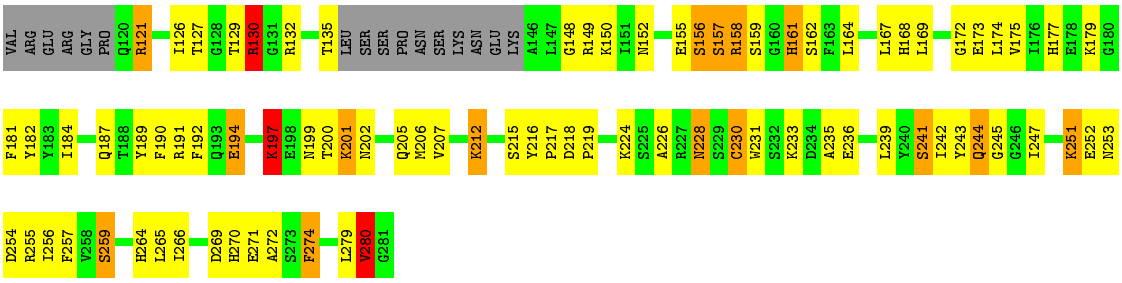




- Molecule 2: TNF-RELATED APOPTOSIS INDUCING LIGAND

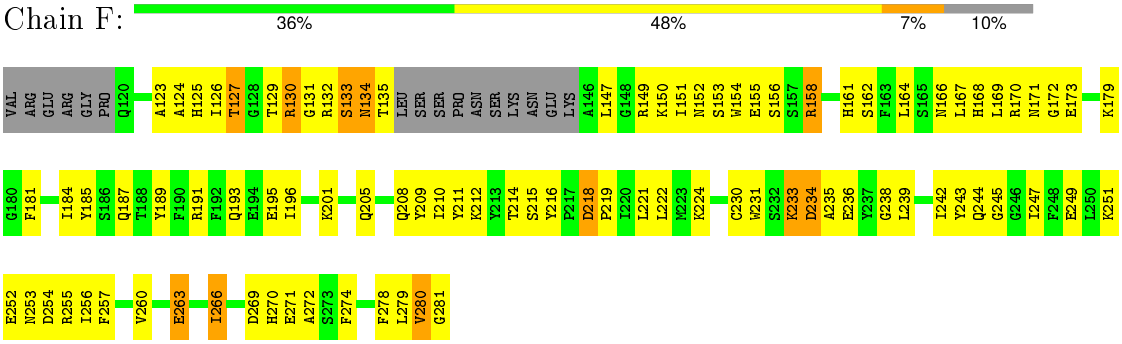
Chain E:





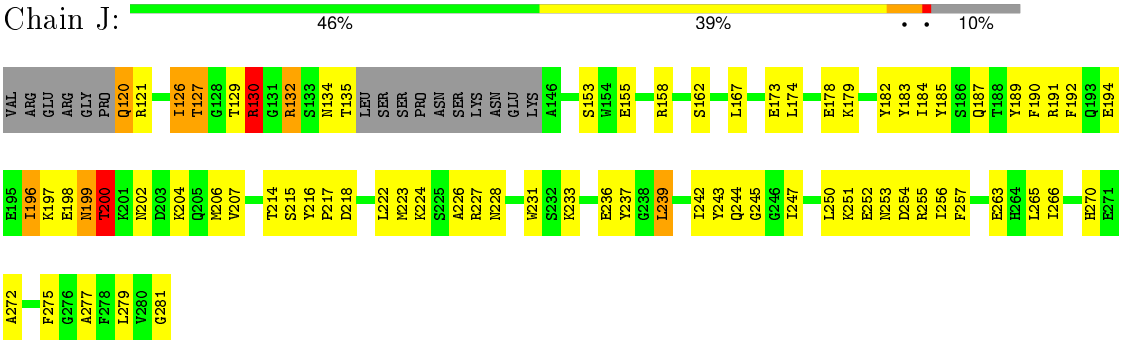
• Molecule 2: TNF-RELATED APOPTOSIS INDUCING LIGAND

Chain F:



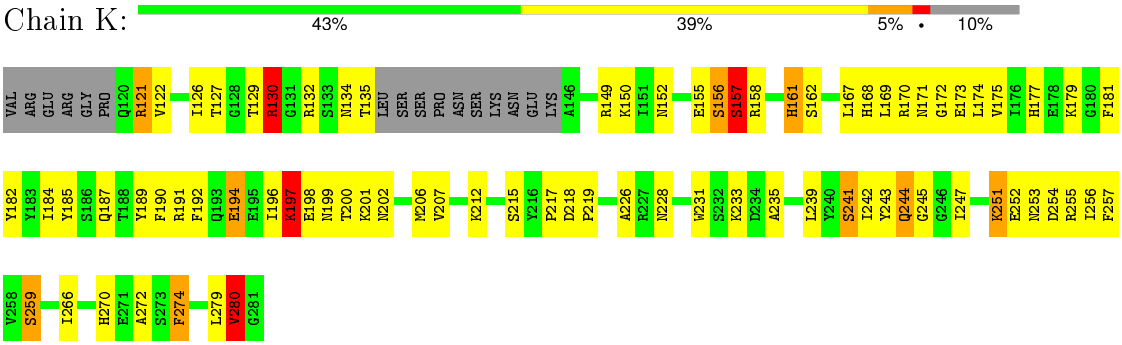
• Molecule 2: TNF-RELATED APOPTOSIS INDUCING LIGAND

Chain J:



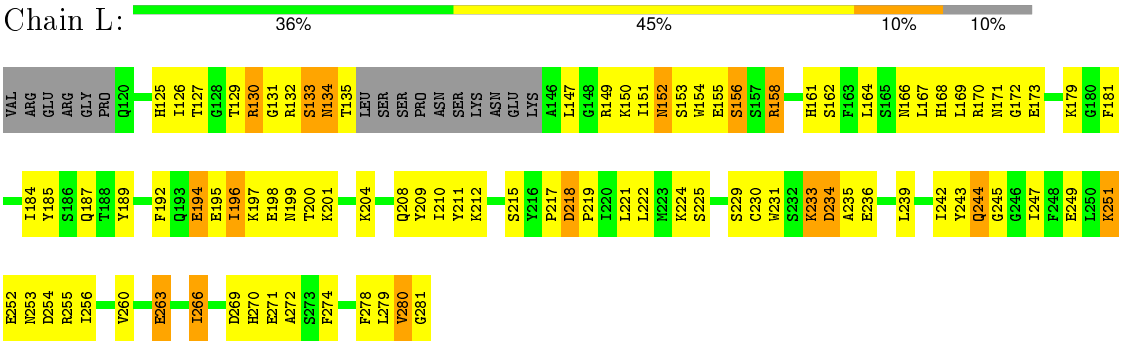
• Molecule 2: TNF-RELATED APOPTOSIS INDUCING LIGAND

Chain K:



• Molecule 2: TNF-RELATED APOPTOSIS INDUCING LIGAND

Chain L:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	68.63Å 124.81Å 128.37Å 90.00° 104.49° 90.00°	Depositor
Resolution (Å)	8.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.20)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.291 , 0.291	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12108	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.56	0/716	0.82	0/969
1	B	2.32	1/849 (0.1%)	1.89	2/1149 (0.2%)
1	C	0.51	0/712	0.72	0/964
1	G	0.62	0/851	0.80	0/1150
1	H	0.58	0/706	0.79	0/957
1	I	0.98	1/716 (0.1%)	1.35	3/969 (0.3%)
2	D	0.86	5/1282 (0.4%)	0.81	1/1724 (0.1%)
2	E	0.61	0/1282	0.79	0/1724
2	F	0.69	1/1276 (0.1%)	0.82	0/1717
2	J	0.62	0/1278	0.78	0/1719
2	K	0.61	0/1282	0.78	0/1724
2	L	0.64	0/1268	0.82	0/1708
All	All	0.89	8/12218 (0.1%)	0.95	6/16474 (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
2	F	0	1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	130	SER	C-O	-64.68	0.00	1.23
1	I	117	CYS	C-N	21.03	1.82	1.34
2	D	198	GLU	CG-CD	13.28	1.71	1.51
2	D	198	GLU	CD-OE1	9.92	1.36	1.25
2	F	191	ARG	C-N	-9.60	1.11	1.34

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	130	SER	CA-C-O	-57.19	0.00	120.10
1	I	117	CYS	O-C-N	-25.30	82.22	122.70
1	I	117	CYS	C-N-CA	17.40	165.20	121.70
1	I	117	CYS	CA-C-N	17.17	154.98	117.20
1	B	127	HIS	O-C-N	-5.34	114.15	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	205	GLN	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	701	0	619	46	0
1	B	833	0	735	75	1
1	C	697	0	613	94	0
1	G	833	0	755	63	0
1	H	691	0	602	55	0
1	I	701	0	618	65	0
2	D	1252	0	1197	79	0
2	E	1252	0	1200	80	0
2	F	1246	0	1188	97	0
2	J	1248	0	1196	72	0
2	K	1252	0	1200	74	0
2	L	1238	0	1172	103	0
3	E	1	0	0	2	0
3	K	1	0	0	1	0
4	A	26	0	0	0	0
4	B	23	0	0	3	2
4	C	6	0	0	2	0
4	D	22	0	0	7	0
4	E	14	0	0	2	0
4	F	13	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	16	0	0	0	1
4	H	7	0	0	0	3
4	I	11	0	0	1	1
4	J	8	0	0	0	0
4	K	9	0	0	1	0
4	L	7	0	0	2	0
All	All	12108	0	11095	768	4

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 768 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:I:117:CYS:C	1:I:118:THR:N	1.82	1.33
1:C:75:PRO:HB3	2:L:170:ARG:HD3	1.30	1.13
1:B:58:LEU:HD23	4:B:3147:HOH:O	1.59	1.02
2:K:202:ASN:HB3	4:K:3043:HOH:O	1.60	1.01
1:C:76:CYS:CB	1:C:82:THR:HG22	1.91	1.00

All (4) 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)
4:B:3160:HOH:O	4:H:3078:HOH:O[1_554]	0.57	1.63
4:G:3053:HOH:O	4:I:3050:HOH:O[2_656]	1.19	1.01
4:B:3160:HOH:O	4:H:3105:HOH:O[1_554]	1.82	0.38
1:B:129:GLU:CG	4:H:3079:HOH:O[1_554]	1.85	0.35

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	86/130 (66%)	77 (90%)	6 (7%)	3 (4%)	4 2
1	B	108/130 (83%)	93 (86%)	12 (11%)	3 (3%)	6 3
1	C	86/130 (66%)	61 (71%)	23 (27%)	2 (2%)	8 4
1	G	106/130 (82%)	90 (85%)	14 (13%)	2 (2%)	10 6
1	H	86/130 (66%)	75 (87%)	9 (10%)	2 (2%)	8 4
1	I	86/130 (66%)	72 (84%)	10 (12%)	4 (5%)	3 1
2	D	148/168 (88%)	132 (89%)	13 (9%)	3 (2%)	9 5
2	E	148/168 (88%)	131 (88%)	12 (8%)	5 (3%)	5 2
2	F	148/168 (88%)	124 (84%)	20 (14%)	4 (3%)	6 3
2	J	148/168 (88%)	132 (89%)	13 (9%)	3 (2%)	9 5
2	K	148/168 (88%)	130 (88%)	13 (9%)	5 (3%)	5 2
2	L	148/168 (88%)	125 (84%)	19 (13%)	4 (3%)	6 3
All	All	1446/1788 (81%)	1242 (86%)	164 (11%)	40 (3%)	6 3

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	130	ARG
2	E	157	SER
2	E	197	LYS
2	E	280	VAL
1	H	25	GLU

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	84/117 (72%)	64 (76%)	20 (24%)	1 0
1	B	97/117 (83%)	76 (78%)	21 (22%)	1 1
1	C	83/117 (71%)	62 (75%)	21 (25%)	1 0
1	G	99/117 (85%)	78 (79%)	21 (21%)	1 1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	82/117 (70%)	61 (74%)	21 (26%)	0 0
1	I	84/117 (72%)	60 (71%)	24 (29%)	0 0
2	D	134/149 (90%)	117 (87%)	17 (13%)	5 4
2	E	134/149 (90%)	111 (83%)	23 (17%)	2 2
2	F	133/149 (89%)	119 (90%)	14 (10%)	8 8
2	J	133/149 (89%)	113 (85%)	20 (15%)	3 3
2	K	134/149 (90%)	114 (85%)	20 (15%)	4 3
2	L	131/149 (88%)	113 (86%)	18 (14%)	4 3
All	All	1328/1596 (83%)	1088 (82%)	240 (18%)	2 1

5 of 240 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	218	ASP
1	G	124	GLU
2	K	280	VAL
2	F	244	GLN
1	G	67	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	270	HIS
1	H	81	ASN
2	L	208	GLN
1	G	32	HIS
1	H	32	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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 (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.