wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 06:22 PM GMT

PDB ID	:	1AFC
Title	:	STRUCTURAL STUDIES OF THE BINDING OF THE ANTI-ULCER DRUG SUCROSE OCTASULFATE TO ACIDIC FIBROBLAST GROWTH FACTOR
Authors	:	Zhu, X.; Hsu, B.T.; Rees, D.C.
Deposited on	:	1993-07-13
Resolution	:	2.70 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:

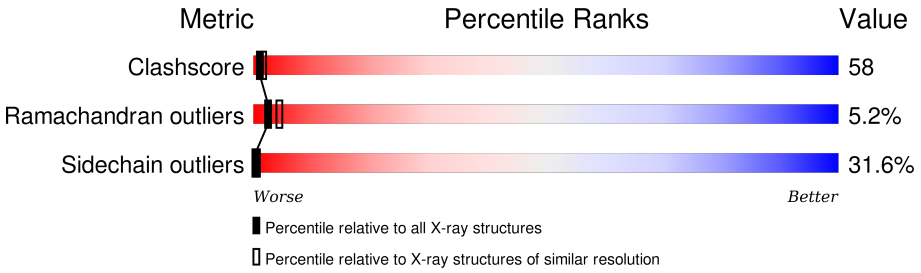
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.70 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	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)

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	140	10% 39% 29% 13% 9%
1	B	140	11% 39% 31% 10% 9%
1	C	140	13% 34% 33% 11% 9%
1	D	140	16% 33% 30% 11% 9%
1	E	140	16% 29% 34% 12% 9%
1	F	140	13% 34% 30% 14% 9%
1	G	140	13% 36% 31% 11% 9%

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Mol	Chain	Length	Quality of chain
1	H	140	11% 33% 28% 19% 9%

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	SCR	A	141	-	-	X	-
2	SCR	D	141	-	-	X	-
2	SCR	E	141	-	-	X	-
2	SCR	G	141	-	-	X	-
2	SCR	H	141	-	-	X	-

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8304 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.

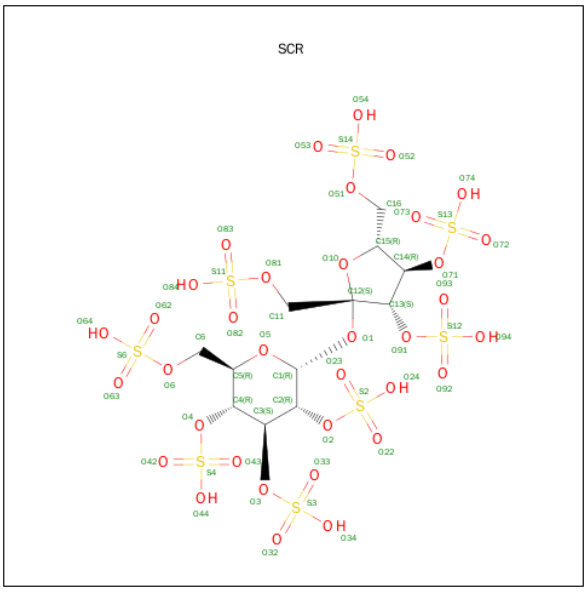
- Molecule 1 is a protein called ACIDIC FIBROBLAST GROWTH FACTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	127	Total	C	N	O	S	0	0	0
			983	630	168	182	3			
1	B	127	Total	C	N	O	S	0	0	0
			983	630	168	182	3			
1	C	127	Total	C	N	O	S	0	0	0
			983	630	168	182	3			
1	D	127	Total	C	N	O	S	0	0	0
			983	630	168	182	3			
1	E	127	Total	C	N	O	S	0	0	0
			983	630	168	182	3			
1	F	127	Total	C	N	O	S	0	0	0
			983	630	168	182	3			
1	G	127	Total	C	N	O	S	0	0	0
			983	630	168	182	3			
1	H	127	Total	C	N	O	S	0	0	0
			983	630	168	182	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	ALA	CYS	CONFLICT	UNP P03968
B	47	ALA	CYS	CONFLICT	UNP P03968
C	47	ALA	CYS	CONFLICT	UNP P03968
D	47	ALA	CYS	CONFLICT	UNP P03968
E	47	ALA	CYS	CONFLICT	UNP P03968
F	47	ALA	CYS	CONFLICT	UNP P03968
G	47	ALA	CYS	CONFLICT	UNP P03968
H	47	ALA	CYS	CONFLICT	UNP P03968

- Molecule 2 is SUGAR (SUCROSE OCTASULFATE) (three-letter code: SCR) (formula: $C_{12}H_{22}O_{35}S_8$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			55	12	35	8		
2	B	1	Total	C	O	S	0	0
			55	12	35	8		
2	C	1	Total	C	O	S	0	0
			55	12	35	8		
2	D	1	Total	C	O	S	0	0
			55	12	35	8		
2	E	1	Total	C	O	S	0	0
			55	12	35	8		
2	F	1	Total	C	O	S	0	0
			55	12	35	8		
2	G	1	Total	C	O	S	0	0
			55	12	35	8		
2	H	1	Total	C	O	S	0	0
			55	12	35	8		

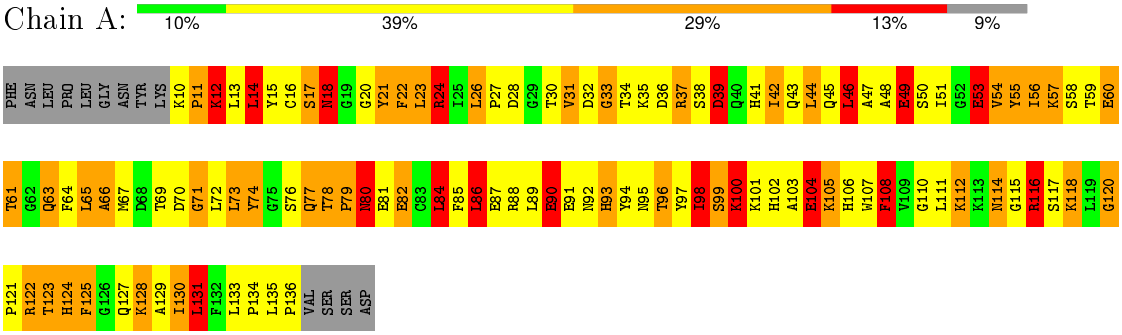
3 Residue-property plots (i)

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.

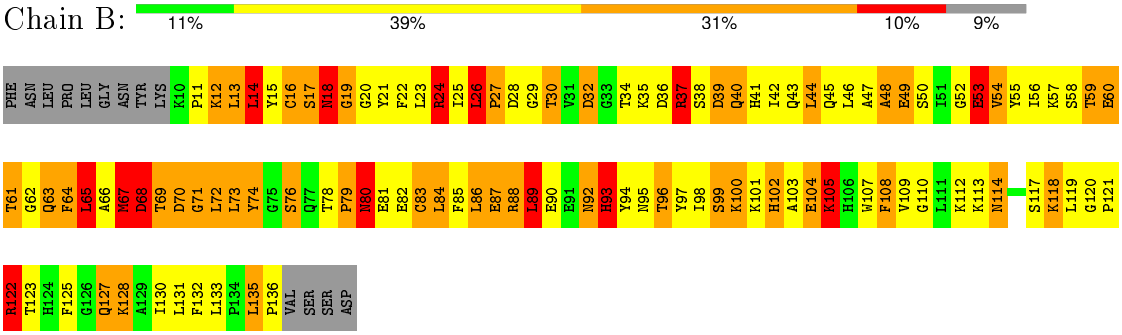
- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR

Chain A:



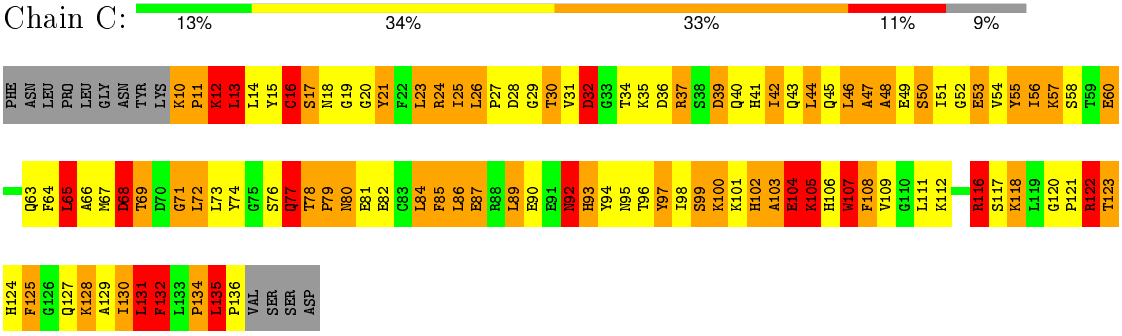
- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR

Chain B:



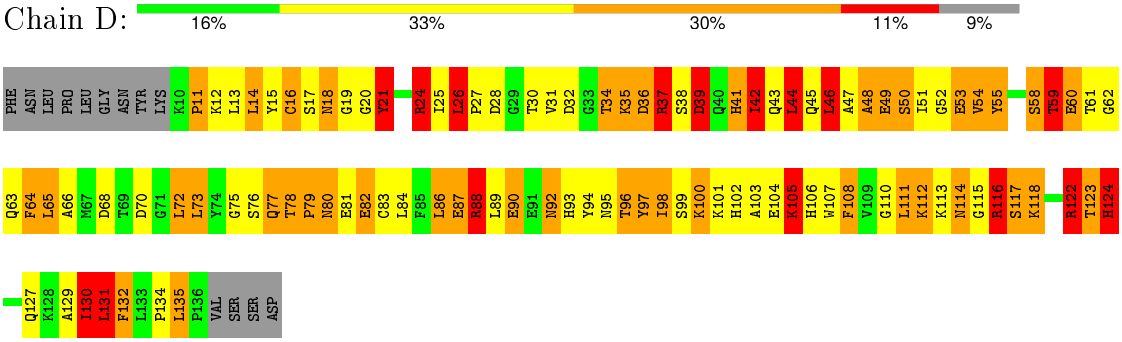
- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR

Chain C:



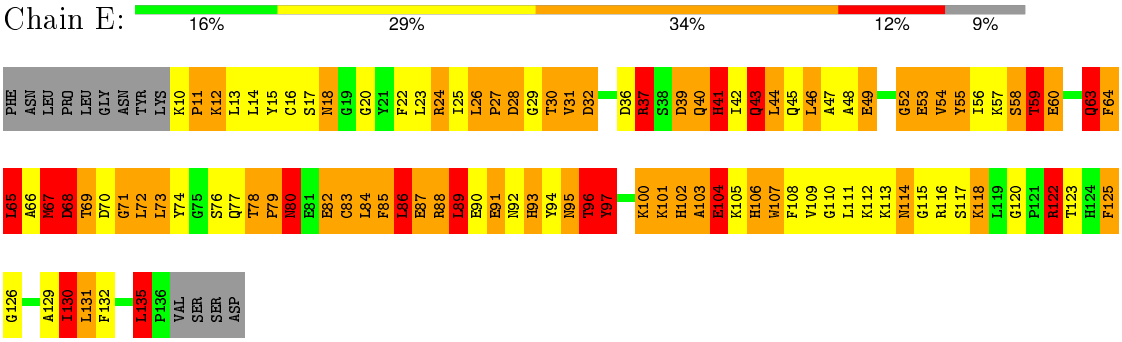
• Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR

Chain D:



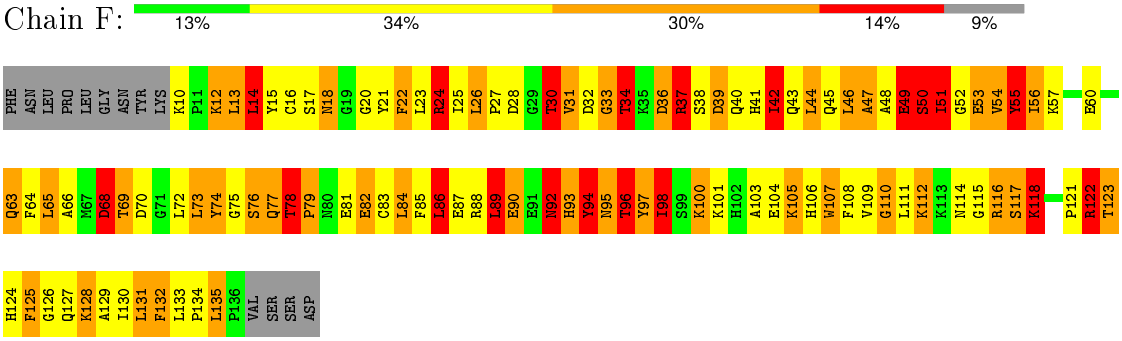
• Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR

Chain E:



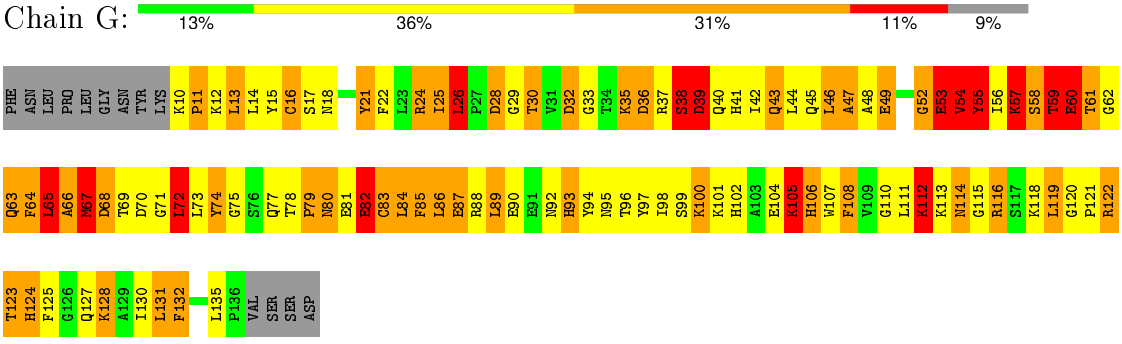
• Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR

Chain F:



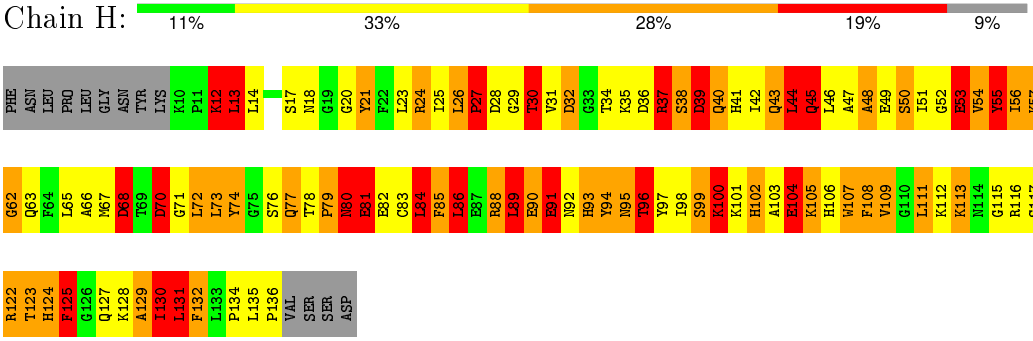
• Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR

Chain G:



• Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR

Chain H:


11%
33%
28%
19%
9%
PHE ASN LEU PRO LEU GLY ASN TYR LYS K10 P11 K12 L13 L14 S17 N18 G19 G20 Y21 F22 L23 R24 I25 L26 P27 D28 G29 T30 V31 D32 G33 T34 K35 D36 R37 S38 D39 Q40 H41 I42 Q43 L44 Q45 L46 A47 A48 E49 S50 I51 G52 E53 V54 Y55 I56 K57 S58 T59 E60 T61
G62 Q63 F64 L65 A66 M67 D68 T69 D70 G71 L72 L73 Y74 G75 S76 Q77 T78 P79 N80 E81 E82 C83 L84 F85 L86 E87 R88 L89 E90 E91 N92 H93 Y94 N95 T96 Y97 I98 S99 K100 K101 H102 A103 E104 K105 H106 W107 F108 V109 G110 L111 K112 K113 N114 G115 R116 S117 K118 L119 G120 P121
R122 T123 H124 F125 G126 Q127 K128 A129 I130 L131 F132 L133 P134 L135 P136 VAL SER SER ASP

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 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	110.60Å 110.60Å 172.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.204 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8304	wwPDB-VP
Average B, all atoms (Å^2)	13.0	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: SCR

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	0.87	0/1007	1.54	8/1363 (0.6%)
1	B	0.91	0/1007	1.48	8/1363 (0.6%)
1	C	0.89	0/1007	1.50	10/1363 (0.7%)
1	D	0.89	0/1007	1.49	11/1363 (0.8%)
1	E	0.91	0/1007	1.49	9/1363 (0.7%)
1	F	0.90	0/1007	1.52	8/1363 (0.6%)
1	G	0.89	0/1007	1.46	4/1363 (0.3%)
1	H	0.90	0/1007	1.51	8/1363 (0.6%)
All	All	0.89	0/8056	1.50	66/10904 (0.6%)

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	89
1	B	0	77
1	C	0	76
1	D	0	76
1	E	0	74
1	F	0	78
1	G	0	67
1	H	0	83
All	All	0	620

There are no bond length outliers.

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	107	TRP	CD1-CG-CD2	11.01	115.11	106.30
1	A	24	ARG	NE-CZ-NH2	-10.65	114.97	120.30
1	D	37	ARG	NE-CZ-NH2	-10.06	115.27	120.30
1	E	24	ARG	NE-CZ-NH2	-9.73	115.43	120.30
1	D	24	ARG	NE-CZ-NH2	-9.52	115.54	120.30

There are no chirality outliers.

5 of 620 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	LYS	Mainchain
1	A	11	PRO	Mainchain
1	A	12	LYS	Mainchain
1	A	14	LEU	Mainchain
1	A	15	TYR	Sidechain

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	983	0	944	109	0
1	B	983	0	944	96	0
1	C	983	0	944	112	0
1	D	983	0	944	96	0
1	E	983	0	944	86	0
1	F	983	0	944	84	0
1	G	983	0	944	126	0
1	H	983	0	944	121	0
2	A	55	0	14	29	0
2	B	55	0	15	11	0
2	C	55	0	14	16	0
2	D	55	0	16	24	0
2	E	55	0	14	26	0
2	F	55	0	14	14	0
2	G	55	0	14	35	0
2	H	55	0	14	23	0
All	All	8304	0	7667	934	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 58.

The worst 5 of 934 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)
2:E:141:SCR:H14	2:E:141:SCR:S14	1.82	1.20
1:A:114:ASN:HD21	1:A:116:ARG:NH1	1.43	1.16
1:G:24:ARG:HH11	1:G:26:LEU:HD11	1.01	1.14
1:H:27:PRO:HB3	1:H:61:THR:HG21	1.31	1.12
1:D:86:LEU:HD21	1:D:100:LYS:HG3	1.30	1.11

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	125/140 (89%)	104 (83%)	17 (14%)	4 (3%)	5	12
1	B	125/140 (89%)	112 (90%)	9 (7%)	4 (3%)	5	12
1	C	125/140 (89%)	103 (82%)	18 (14%)	4 (3%)	5	12
1	D	125/140 (89%)	104 (83%)	16 (13%)	5 (4%)	4	8
1	E	125/140 (89%)	102 (82%)	16 (13%)	7 (6%)	2	3
1	F	125/140 (89%)	105 (84%)	11 (9%)	9 (7%)	1	1
1	G	125/140 (89%)	105 (84%)	15 (12%)	5 (4%)	4	8
1	H	125/140 (89%)	92 (74%)	19 (15%)	14 (11%)	0	0
All	All	1000/1120 (89%)	827 (83%)	121 (12%)	52 (5%)	2	4

5 of 52 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	ASN

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Mol	Chain	Res	Type
1	A	81	GLU
1	B	18	ASN
1	B	68	ASP
1	D	18	ASN

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	101/122 (83%)	69 (68%)	32 (32%)	0	0
1	B	101/122 (83%)	68 (67%)	33 (33%)	0	0
1	C	101/122 (83%)	67 (66%)	34 (34%)	0	0
1	D	101/122 (83%)	74 (73%)	27 (27%)	0	2
1	E	101/122 (83%)	69 (68%)	32 (32%)	0	0
1	F	101/122 (83%)	71 (70%)	30 (30%)	0	1
1	G	101/122 (83%)	64 (63%)	37 (37%)	0	0
1	H	101/122 (83%)	71 (70%)	30 (30%)	0	1
All	All	808/976 (83%)	553 (68%)	255 (32%)	0	0

5 of 255 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	84	LEU
1	E	78	THR
1	H	55	TYR
1	D	105	LYS
1	E	37	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	106	HIS

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Mol	Chain	Res	Type
1	E	95	ASN
1	H	80	ASN
1	E	43	GLN
1	E	63	GLN

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

8 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	SCR	A	141	-	56,56,56	1.67	10 (17%)	79,92,92	1.55	14 (17%)
2	SCR	B	141	-	56,56,56	1.52	9 (16%)	79,92,92	1.28	9 (11%)
2	SCR	C	141	-	56,56,56	1.52	9 (16%)	79,92,92	1.61	11 (13%)
2	SCR	D	141	-	56,56,56	1.57	9 (16%)	79,92,92	1.37	8 (10%)
2	SCR	E	141	-	56,56,56	1.57	10 (17%)	79,92,92	1.66	12 (15%)
2	SCR	F	141	-	56,56,56	1.44	10 (17%)	79,92,92	1.17	6 (7%)
2	SCR	G	141	-	56,56,56	1.32	8 (14%)	79,92,92	1.79	15 (18%)
2	SCR	H	141	-	56,56,56	1.59	8 (14%)	79,92,92	1.58	12 (15%)

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	SCR	A	141	-	-	0/48/88/88	0/2/2/2
2	SCR	B	141	-	-	0/48/88/88	0/2/2/2
2	SCR	C	141	-	-	0/48/88/88	0/2/2/2
2	SCR	D	141	-	-	0/48/88/88	0/2/2/2
2	SCR	E	141	-	-	0/48/88/88	0/2/2/2
2	SCR	F	141	-	-	0/48/88/88	0/2/2/2
2	SCR	G	141	-	-	1/48/88/88	0/2/2/2
2	SCR	H	141	-	-	0/48/88/88	0/2/2/2

The worst 5 of 73 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	141	SCR	O91-S12	-5.52	1.39	1.57
2	B	141	SCR	O91-S12	-4.53	1.42	1.57
2	H	141	SCR	O4-S4	-4.49	1.42	1.57
2	H	141	SCR	O2-S2	-4.35	1.43	1.57
2	H	141	SCR	O91-S12	-4.29	1.43	1.57

The worst 5 of 87 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	141	SCR	C1-O5-C5	-6.43	101.27	113.75
2	H	141	SCR	O2-C2-C1	-5.44	100.25	107.65
2	D	141	SCR	O4-C4-C3	-5.37	96.61	108.48
2	H	141	SCR	C14-O71-S13	-4.95	109.35	118.77
2	E	141	SCR	C1-O5-C5	-4.83	104.38	113.75

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	141	SCR	S4-O4-C4-C5

There are no ring outliers.

8 monomers are involved in 178 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	141	SCR	29	0
2	B	141	SCR	11	0
2	C	141	SCR	16	0
2	D	141	SCR	24	0
2	E	141	SCR	26	0
2	F	141	SCR	14	0
2	G	141	SCR	35	0
2	H	141	SCR	23	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.