WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 20, 2023 – 10:50 AM EDT

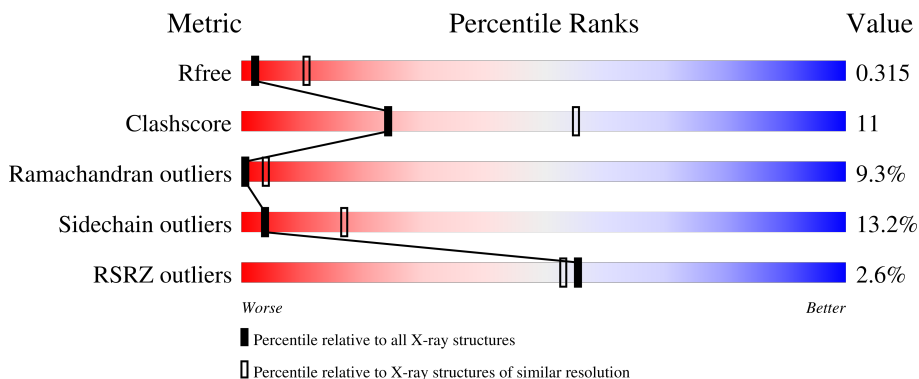|		
PDB ID	:	5IHL
Title	:	STRUCTURE OF THE EXTRACELLULAR DOMAIN OF THE CD40 IN COMPLEX WITH 3H56-5 DAB
Authors	:	Sheriff, S.
Deposited on	:	2016-02-29
Resolution	:	3.30 Å(reported)

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 3.30 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.
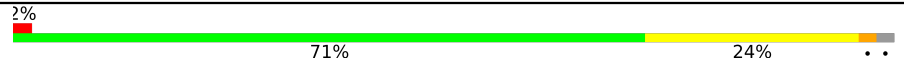
Metric	Percentile Ranks	Value
Rfree		0.315
Clashscore		11
Ramachandran outliers		9.3%
Sidechain outliers		13.2%
RSRZ outliers		2.6%

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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	183	% / 51% 30% 10% · 8%
1	D	183	5% / 56% 28% 5% · 10%
1	F	183	4% / 56% 26% 6% · 10%
1	H	183	4% / 57% 23% 9% · 9%
2	B	121	71% 22% · ·

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Mol	Chain	Length	Quality of chain
2	E	121	2% 71% 24%
2	G	121	74% 20%
2	I	121	2% 68% 28%

2   Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 8291 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 Tumor necrosis factor receptor superfamily member 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	168	Total	C	N	O	S	0	0	0
			1224	744	207	253	20			
1	D	165	Total	C	N	O	S	0	0	0
			1130	677	199	234	20			
1	F	165	Total	C	N	O	S	0	0	0
			1178	722	199	237	20			
1	H	167	Total	C	N	O	S	0	0	0
			1164	705	201	238	20			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	ASP	ASN	SEE REMARK 999	UNP P25942
A	180	ASP	ASN	SEE REMARK 999	UNP P25942
A	194	ASP	-	expression tag	UNP P25942
A	195	PRO	-	expression tag	UNP P25942
A	196	GLY	-	expression tag	UNP P25942
A	197	GLY	-	expression tag	UNP P25942
A	198	GLY	-	expression tag	UNP P25942
A	199	GLY	-	expression tag	UNP P25942
A	200	GLY	-	expression tag	UNP P25942
A	201	ARG	-	expression tag	UNP P25942
A	202	LEU	-	expression tag	UNP P25942
A	203	VAL	-	expression tag	UNP P25942
A	204	PRO	-	expression tag	UNP P25942
A	205	ARG	-	expression tag	UNP P25942
D	153	ASP	ASN	SEE REMARK 999	UNP P25942
D	180	ASP	ASN	SEE REMARK 999	UNP P25942
D	194	ASP	-	expression tag	UNP P25942
D	195	PRO	-	expression tag	UNP P25942
D	196	GLY	-	expression tag	UNP P25942
D	197	GLY	-	expression tag	UNP P25942
D	198	GLY	-	expression tag	UNP P25942

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Chain	Residue	Modelled	Actual	Comment	Reference
D	199	GLY	-	expression tag	UNP P25942
D	200	GLY	-	expression tag	UNP P25942
D	201	ARG	-	expression tag	UNP P25942
D	202	LEU	-	expression tag	UNP P25942
D	203	VAL	-	expression tag	UNP P25942
D	204	PRO	-	expression tag	UNP P25942
D	205	ARG	-	expression tag	UNP P25942
F	153	ASP	ASN	SEE REMARK 999	UNP P25942
F	180	ASP	ASN	SEE REMARK 999	UNP P25942
F	194	ASP	-	expression tag	UNP P25942
F	195	PRO	-	expression tag	UNP P25942
F	196	GLY	-	expression tag	UNP P25942
F	197	GLY	-	expression tag	UNP P25942
F	198	GLY	-	expression tag	UNP P25942
F	199	GLY	-	expression tag	UNP P25942
F	200	GLY	-	expression tag	UNP P25942
F	201	ARG	-	expression tag	UNP P25942
F	202	LEU	-	expression tag	UNP P25942
F	203	VAL	-	expression tag	UNP P25942
F	204	PRO	-	expression tag	UNP P25942
F	205	ARG	-	expression tag	UNP P25942
H	153	ASP	ASN	SEE REMARK 999	UNP P25942
H	180	ASP	ASN	SEE REMARK 999	UNP P25942
H	194	ASP	-	expression tag	UNP P25942
H	195	PRO	-	expression tag	UNP P25942
H	196	GLY	-	expression tag	UNP P25942
H	197	GLY	-	expression tag	UNP P25942
H	198	GLY	-	expression tag	UNP P25942
H	199	GLY	-	expression tag	UNP P25942
H	200	GLY	-	expression tag	UNP P25942
H	201	ARG	-	expression tag	UNP P25942
H	202	LEU	-	expression tag	UNP P25942
H	203	VAL	-	expression tag	UNP P25942
H	204	PRO	-	expression tag	UNP P25942
H	205	ARG	-	expression tag	UNP P25942

- Molecule 2 is a protein called 3H56-5 domain antibody (dAb).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	117	Total 893	C 563	N 151	O 174	S 5	0	0	0
2	E	118	Total 889	C 562	N 149	O 173	S 5	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	117	Total 895	C 566	N 152	O 172	S 5	0	0	0
2	I	117	Total 898	C 566	N 152	O 175	S 5	0	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 5	O 4	S 1	0	0
3	A	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	G	1	Total 5	O 4	S 1	0	0

3 Residue-property plots ⓘ
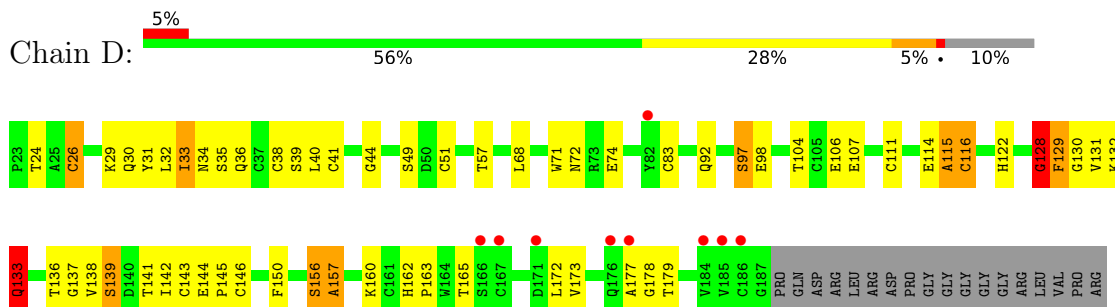
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.
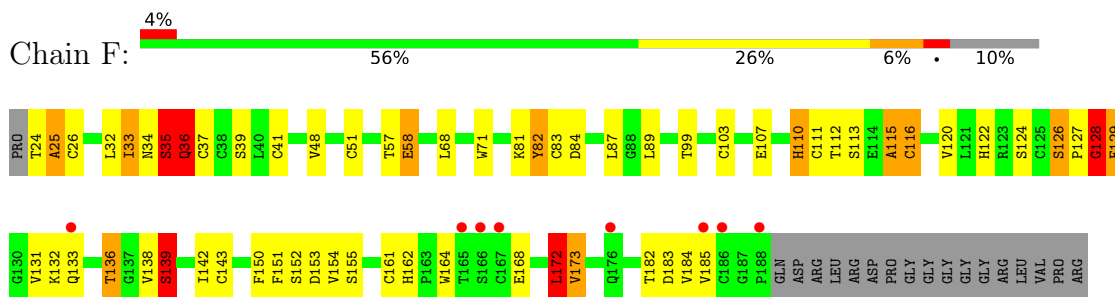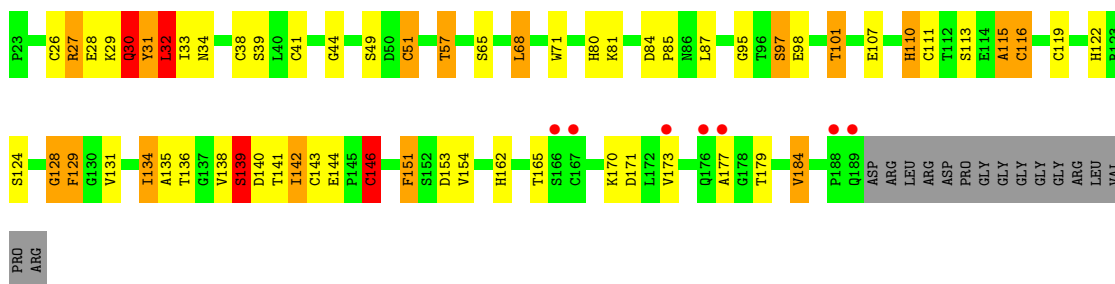
• Molecule 1: Tumor necrosis factor receptor superfamily member 5

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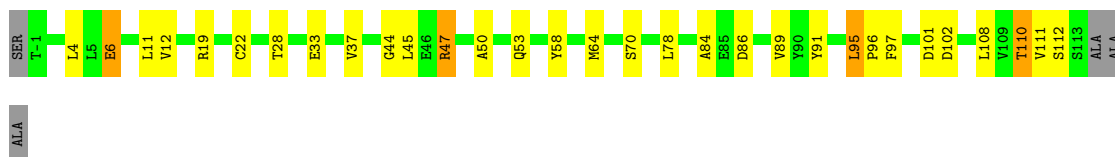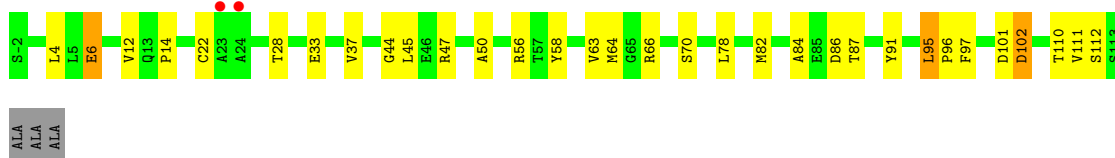• Molecule 1: Tumor necrosis factor receptor superfamily member 5

• Molecule 1: Tumor necrosis factor receptor superfamily member 5

P23 C26 R27 E28 K29 Q30 Y31 L32 I33 N34 C38 S39 L40 C41 G44 S49 D50 C51 T57 S65 L68 W71 H80 K81 D84 P85 N86 L87 G95 T96 S97 E98 T101 E107 H110 C111 T112 S113 E114 A115 C116 C119 H122 R123

S124 G128 F129 G130 V131 I134 A135 T136 G137 V138 S139 D140 T141 I142 C143 E144 P145 C146 F151 S152 D153 V154 H162 T165 S166 C167 K170 D171 L172 V173 Q176 A177 G178 T179 V184 P188 Q189 ASP ARG LEU ARG ASP PRO GLY GLY GLY ARG LEU VAL

PRO ARG

- Molecule 2: 3H56-5 domain antibody (dAb)

Chain B:
71%   22%

SER T-1 L4 L5 E6 L11 V12 R19 C22 T28 E33 V37 G44 L45 E46 R47 A50 Q53 Y58 M64 S70 L78 A84 E85 D86 V89 Y90 Y91 L95 P96 F97 D101 D102 L108 V109 T110 V111 S112 S113 ALA ALA

ALA

- Molecule 2: 3H56-5 domain antibody (dAb)

Chain E:
2%
71%   24%

S-2 L4 L5 E6 V12 Q13 P14 C22 A23 A24 T28 E33 V37 G44 L45 E46 R47 A50 R56 T57 Y58 V63 M64 G65 R66 S70 L78 M82 A84 E85 D86 T87 Y91 L95 P96 F97 D101 D102 T110 V111 S112 S113

ALA ALA ALA

- Molecule 2: 3H56-5 domain antibody (dAb)

Chain G:
74%   20%

SER T-1 L4 L5 E6 C22 R30 V37 G44 L45 E46 R47 A50 R56 T57 Y58 V63 M64 G65 R66 S70 N73 L78 D86 T87 Y91 L95 P96 F97 D101 D102 T107 T110 V111 S112 S113 ALA ALA ALA

- Molecule 2: 3H56-5 domain antibody (dAb)

Chain I:
2%
68%   28%

SER T-1 E6 S7 V12 Q13 P14 C22 A23 A24 T28 F29 R30 D31 A40 K43 G44 L45 A50 P52A R56 T57 Y58 V63 M64 G65 R66 S70 N73 L78 M82 T87 A88 V89 Y90 Y91 L95 F99 D101 D102 T107 L108

V109 T110 V111 S112 S113 ALA ALA ALA

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	156.60Å 158.30Å 200.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.04 – 3.30 29.04 – 3.30	Depositor EDS
% Data completeness (in resolution range)	90.8 (29.04-3.30) 90.8 (29.04-3.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	9.03 (at 3.31Å)	Xtriage
Refinement program	BUSTER 2.11.6	Depositor
R, R_{free}	0.268 , 0.298 0.275 , 0.315	Depositor DCC
R_{free} test set	953 reflections (2.78%)	wwPDB-VP
Wilson B-factor (Å^2)	62.4	Xtriage
Anisotropy	0.603	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 63.3	EDS
L-test for twinning[2]	$< |L| > = 0.52, < L^2 > = 0.37$	Xtriage
Estimated twinning fraction	0.085 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	8291	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.70 % 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 9.0061e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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: SO4

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	0.68	0/1252	0.97	3/1708 (0.2%)
1	D	0.53	0/1152	0.94	4/1576 (0.3%)
1	F	0.52	0/1205	0.91	4/1648 (0.2%)
1	H	0.56	0/1188	0.95	4/1622 (0.2%)
2	B	0.48	0/913	0.76	0/1242
2	E	0.44	0/909	0.73	0/1237
2	G	0.43	0/915	0.74	0/1242
2	I	0.46	0/918	0.71	0/1246
All	All	0.53	0/8452	0.86	15/11521 (0.1%)

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	156	SER	C-N-CA	6.70	138.46	121.70
1	A	138	VAL	C-N-CA	6.29	137.42	121.70
1	H	128	GLY	C-N-CA	6.23	137.27	121.70
1	D	34	ASN	C-N-CA	5.97	136.63	121.70
1	D	128	GLY	C-N-CA	5.84	136.29	121.70

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	1224	0	1035	32	0
1	D	1130	0	891	25	0
1	F	1178	0	986	33	0
1	H	1164	0	957	32	0
2	B	893	0	833	14	0
2	E	889	0	831	18	0
2	G	895	0	844	13	0
2	I	898	0	847	15	0
3	A	10	0	0	0	0
3	B	5	0	0	0	0
3	G	5	0	0	0	0
All	All	8291	0	7224	170	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 11.

The worst 5 of 170 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:B:84:ALA:HA	2:B:111:VAL:HG21	1.34	1.04
2:E:84:ALA:HA	2:E:111:VAL:HG21	1.54	0.90
1:F:35:SER:HA	1:F:36:GLN:O	1.82	0.80
1:F:128:GLY:HA3	1:F:129:PHE:HB2	1.68	0.76
1:D:136:THR:HA	1:D:138:VAL:N	2.00	0.76

There are no symmetry-related clashes.

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	166/183 (91%)	120 (72%)	21 (13%)	25 (15%)	0	1
1	D	163/183 (89%)	111 (68%)	31 (19%)	21 (13%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	163/183 (89%)	115 (71%)	26 (16%)	22 (14%)	0	1
1	H	165/183 (90%)	120 (73%)	23 (14%)	22 (13%)	0	1
2	B	115/121 (95%)	102 (89%)	9 (8%)	4 (4%)	3	21
2	E	116/121 (96%)	105 (90%)	9 (8%)	2 (2%)	9	35
2	G	115/121 (95%)	103 (90%)	7 (6%)	5 (4%)	2	16
2	I	115/121 (95%)	105 (91%)	7 (6%)	3 (3%)	5	27
All	All	1118/1216 (92%)	881 (79%)	133 (12%)	104 (9%)	0	4

5 of 104 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	SER
1	A	154	VAL
1	A	168	GLU
1	A	179	THR
1	A	185	VAL

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	132/162 (82%)	112 (85%)	20 (15%)	3	13
1	D	109/162 (67%)	95 (87%)	14 (13%)	4	18
1	F	122/162 (75%)	105 (86%)	17 (14%)	3	16
1	H	117/162 (72%)	97 (83%)	20 (17%)	2	9
2	B	91/98 (93%)	79 (87%)	12 (13%)	4	17
2	E	90/98 (92%)	79 (88%)	11 (12%)	5	20
2	G	91/98 (93%)	83 (91%)	8 (9%)	10	33
2	I	92/98 (94%)	83 (90%)	9 (10%)	8	29
All	All	844/1040 (81%)	733 (87%)	111 (13%)	4	17

5 of 111 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	26	CYS
2	I	101	ASP
1	F	139	SER
2	I	95	LEU
1	H	142	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	162	HIS
1	H	122	HIS

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 monosaccharides in this entry.

5.6   Ligand geometry ⓘ

4 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	#$|Z| > 2$
3	SO4	B	201	-	4,4,4	0.18	0	6,6,6	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\|$ > 2	Counts	RMSZ	#$\|Z\|$ > 2
3	SO4	A	302	-	4,4,4	0.24	0	6,6,6	0.33	0
3	SO4	G	201	-	4,4,4	0.14	0	6,6,6	0.20	0
3	SO4	A	301	-	4,4,4	0.24	0	6,6,6	0.40	0

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 ⓘ

There are no such residues in this entry.

5.8   Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	168/183 (91%)	-0.09	2 (1%)	79	78	27, 59, 94, 132	0
1	D	165/183 (90%)	0.17	9 (5%)	25	23	45, 93, 153, 167	0
1	F	165/183 (90%)	0.21	8 (4%)	30	28	39, 88, 176, 183	0
1	H	167/183 (91%)	0.08	7 (4%)	36	34	31, 88, 174, 182	0
2	B	117/121 (96%)	-0.28	0	100	100	20, 60, 86, 113	0
2	E	118/121 (97%)	-0.05	2 (1%)	70	68	60, 86, 123, 149	0
2	G	117/121 (96%)	-0.22	0	100	100	38, 68, 109, 136	0
2	I	117/121 (96%)	-0.27	2 (1%)	70	68	32, 63, 110, 123	0
All	All	1134/1216 (93%)	-0.03	30 (2%)	56	53	20, 77, 149, 183	0

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	189	GLN	4.6
1	H	176	GLN	4.2
1	F	166	SER	3.7
1	H	177	ALA	3.7
1	D	184	VAL	3.7

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.

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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. 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(Å^2)	Q<0.9
3	SO4	A	302	5/5	0.93	0.18	92,93,96,101	0
3	SO4	G	201	5/5	0.94	0.12	115,117,120,123	0
3	SO4	A	301	5/5	0.95	0.18	50,51,55,56	0
3	SO4	B	201	5/5	0.96	0.14	94,98,99,105	0

6.5 Other polymers (i)

There are no such residues in this entry.