



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:35 AM UTC

PDB ID : 7ST5 / pdb_00007st5
Title : Structure of Fab CC-95251 in complex with SIRP-alpha
Authors : Fenalti, G.
Deposited on : 2021-11-12
Resolution : 2.20 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

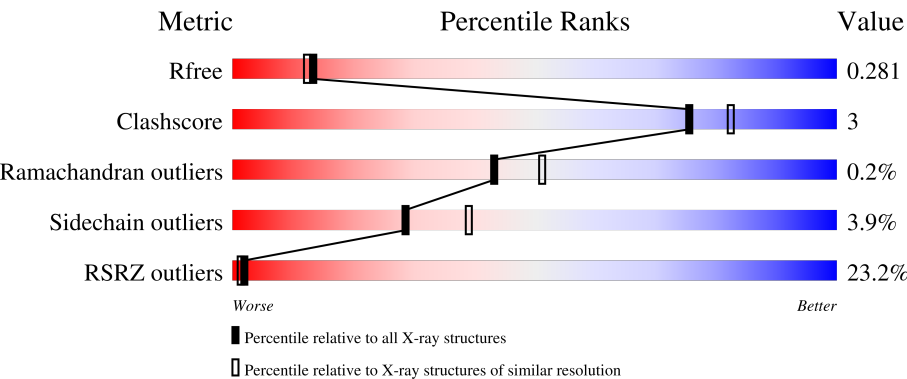
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 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 $\leq 5\%$. 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	H	227	12% 84% 7% 9%
1	h	227	21% 86% • 9%
2	L	214	11% 89% 9% •
2	l	214	16% 86% 12% •
3	A	125	39% 69% 14% 17%

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Mol	Chain	Length	Quality of chain
3	F	125	47% 63% 18% • 18%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7644 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 Fab CC-95251 anti-SIRP-alpha heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	206	Total	C	N	O	S	0	0	0
			1487	943	249	288	7			
1	h	206	Total	C	N	O	S	0	0	0
			1465	929	247	282	7			

- Molecule 2 is a protein called Fab CC-95251 anti-SIRP-alpha light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	211	Total	C	N	O	S	0	0	0
			1510	955	254	296	5			
2	l	211	Total	C	N	O	S	0	0	0
			1473	938	247	284	4			

- Molecule 3 is a protein called Tyrosine-protein phosphatase non-receptor type substrate 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	102	Total	C	N	O	S	0	0	0
			750	476	133	138	3			
3	A	104	Total	C	N	O	S	0	0	0
			761	482	137	139	3			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	120	SER	-	expression tag	UNP P78324
F	121	GLY	-	expression tag	UNP P78324
F	122	LEU	-	expression tag	UNP P78324
F	123	VAL	-	expression tag	UNP P78324
F	124	PRO	-	expression tag	UNP P78324
F	125	ARG	-	expression tag	UNP P78324
A	120	SER	-	expression tag	UNP P78324
A	121	GLY	-	expression tag	UNP P78324

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Chain	Residue	Modelled	Actual	Comment	Reference
A	122	LEU	-	expression tag	UNP P78324
A	123	VAL	-	expression tag	UNP P78324
A	124	PRO	-	expression tag	UNP P78324
A	125	ARG	-	expression tag	UNP P78324

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	1	1	Total C O 4 2 2	0	0
4	1	1	Total C O 4 2 2	0	0
4	1	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	L	1	Total	C	O	0	0
			6	3	3		

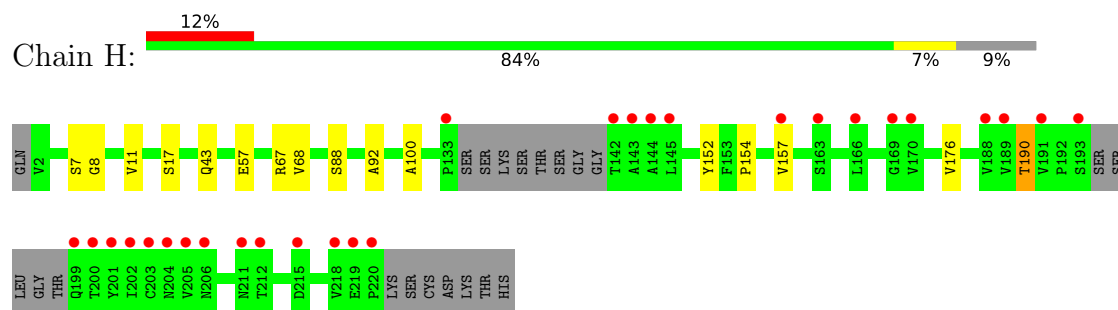
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	44	Total	O	0	0
			44	44		
6	L	29	Total	O	0	0
			29	29		
6	F	18	Total	O	0	0
			18	18		
6	h	34	Total	O	0	0
			34	34		
6	l	26	Total	O	0	0
			26	26		
6	A	17	Total	O	0	0
			17	17		

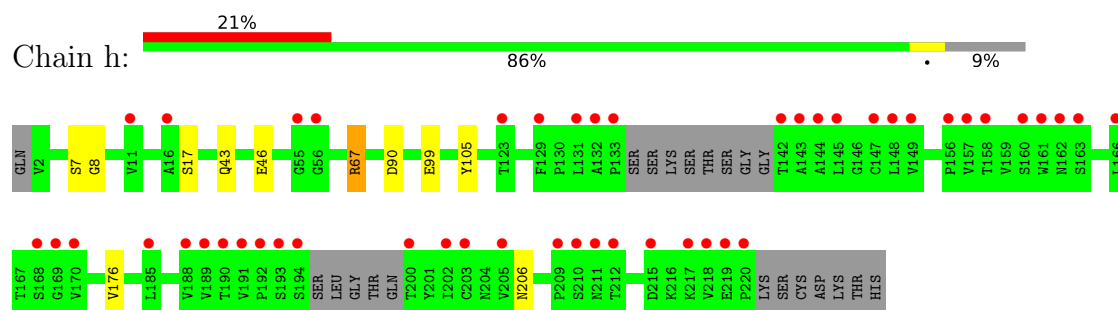
3 Residue-property plots

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.

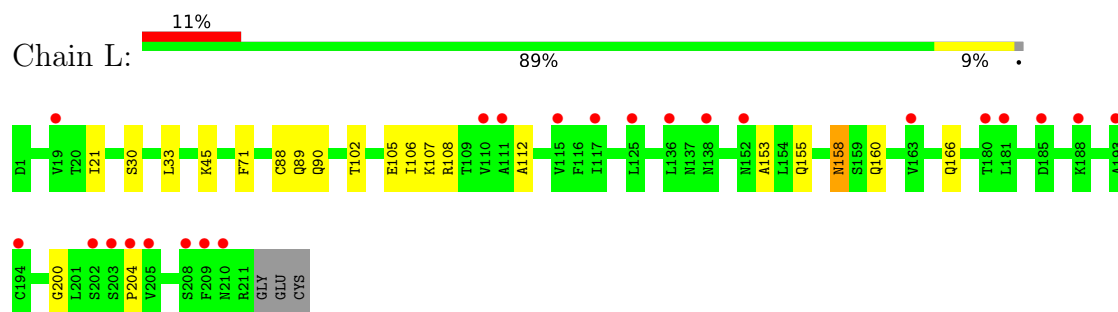
- Molecule 1: Fab CC-95251 anti-SIRP-alpha heavy chain



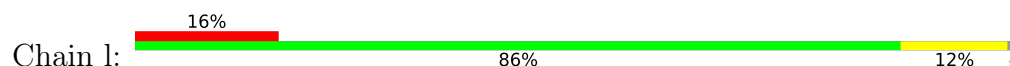
- Molecule 1: Fab CC-95251 anti-SIRP-alpha heavy chain

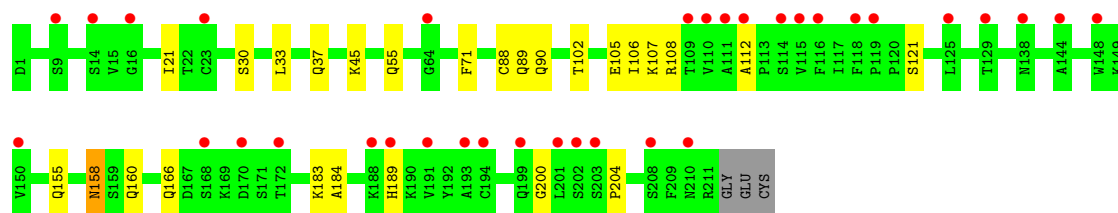


- Molecule 2: Fab CC-95251 anti-SIRP-alpha light chain

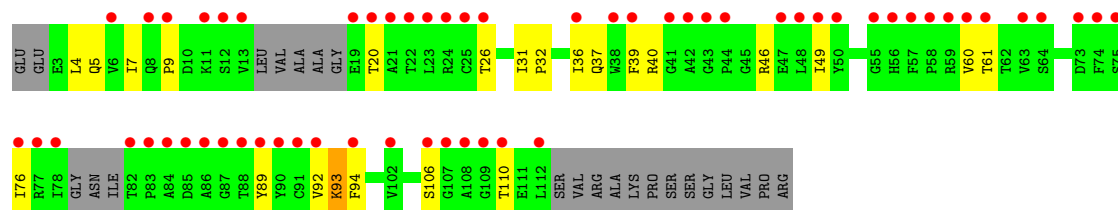


- Molecule 2: Fab CC-95251 anti-SIRP-alpha light chain

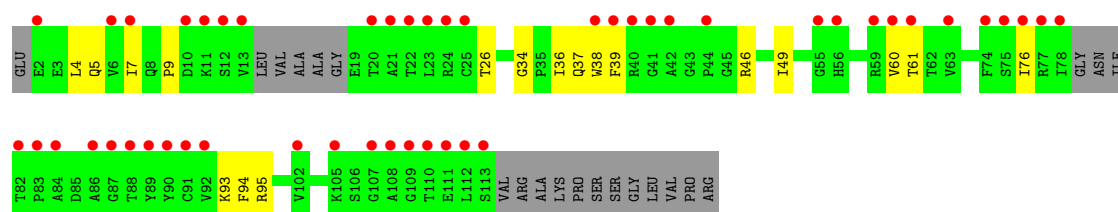




● Molecule 3: Tyrosine-protein phosphatase non-receptor type substrate 1



● Molecule 3: Tyrosine-protein phosphatase non-receptor type substrate 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	42.96Å 97.70Å 103.39Å 77.18° 85.92° 85.74°	Depositor
Resolution (Å)	50.01 – 2.20 50.01 – 2.20	Depositor EDS
% Data completeness (in resolution range)	88.2 (50.01-2.20) 88.2 (50.01-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.245 , 0.280 0.249 , 0.281	Depositor DCC
R_{free} test set	3601 reflections (4.34%)	wwPDB-VP
Wilson B-factor (Å ²)	37.3	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7644	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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

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	H	1.11	2/1522 (0.1%)	1.05	3/2081 (0.1%)
1	h	1.13	1/1500 (0.1%)	1.04	4/2050 (0.2%)
2	L	1.13	2/1545 (0.1%)	1.07	1/2117 (0.0%)
2	l	1.11	2/1508 (0.1%)	1.07	2/2070 (0.1%)
3	A	1.06	0/775	1.12	0/1049
3	F	1.06	1/765 (0.1%)	1.11	1/1039 (0.1%)
All	All	1.11	8/7615 (0.1%)	1.07	11/10406 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	93	LYS	CA-C	-6.36	1.45	1.52
2	l	45	LYS	C-O	-6.00	1.16	1.23
1	H	92	ALA	CA-C	-5.96	1.45	1.52
2	L	45	LYS	C-O	-5.65	1.17	1.23
1	h	46	GLU	C-O	5.43	1.30	1.24
1	H	68	VAL	C-O	-5.38	1.18	1.24
2	L	153	ALA	CA-C	5.04	1.59	1.52
2	l	37	GLN	C-O	-5.04	1.18	1.24

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	8	GLY	N-CA-C	6.31	122.16	112.51
1	h	8	GLY	N-CA-C	5.87	121.49	112.51
1	h	90	ASP	N-CA-C	-5.60	106.12	113.17
1	H	67	ARG	NE-CZ-NH1	-5.50	116.00	121.50
1	H	67	ARG	NE-CZ-NH2	5.39	124.06	119.20
2	L	108	ARG	NE-CZ-NH2	5.30	123.97	119.20
2	l	189	HIS	N-CA-C	-5.25	101.43	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	76	ILE	N-CA-C	5.21	115.98	108.48
1	h	67	ARG	NE-CZ-NH2	5.11	123.80	119.20
2	l	108	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	h	67	ARG	NE-CZ-NH1	-5.03	116.47	121.50

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	H	1487	0	1347	6	0
1	h	1465	0	1286	3	0
2	L	1510	0	1355	7	0
2	l	1473	0	1269	9	0
3	A	761	0	709	9	0
3	F	750	0	703	11	0
4	A	4	0	6	0	0
4	F	4	0	6	0	0
4	H	4	0	6	0	0
4	l	12	0	18	0	0
5	L	6	0	8	0	0
6	A	17	0	0	0	0
6	F	18	0	0	2	0
6	H	44	0	0	1	0
6	L	29	0	0	0	0
6	h	34	0	0	1	0
6	l	26	0	0	1	0
All	All	7644	0	6713	42	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 3.

All (42) 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:H:100:ALA:HB3	6:H:407:HOH:O	1.89	0.71
2:L:155:GLN:HB3	2:L:158:ASN:HD21	1.62	0.64
3:F:89:TYR:HB2	6:F:309:HOH:O	1.96	0.64
2:l:155:GLN:HB3	2:l:158:ASN:HD21	1.64	0.63
2:L:33:LEU:HD22	2:L:71:PHE:CG	2.41	0.56
2:l:33:LEU:HD22	2:l:71:PHE:CG	2.41	0.54
3:A:36:ILE:HD13	3:A:93:LYS:HA	1.90	0.54
1:h:176:VAL:HG21	2:l:160:GLN:HB3	1.88	0.54
3:F:110:THR:HB	6:F:309:HOH:O	2.06	0.54
1:H:176:VAL:HG21	2:L:160:GLN:HB3	1.89	0.53
3:F:36:ILE:HD13	3:F:93:LYS:HA	1.92	0.52
2:L:106:ILE:H	2:L:166:GLN:HE22	1.57	0.52
3:F:40:ARG:N	3:F:49:ILE:HD11	2.26	0.51
2:l:121:SER:CB	6:l:409:HOH:O	2.58	0.51
1:h:67:ARG:HD3	6:h:303:HOH:O	2.10	0.51
3:F:37:GLN:HB2	3:F:94:PHE:CE1	2.47	0.49
2:l:21:ILE:HG12	2:l:102:THR:HG21	1.94	0.49
3:A:37:GLN:HB2	3:A:94:PHE:CE1	2.48	0.49
2:L:21:ILE:HG12	2:L:102:THR:HG21	1.95	0.48
3:A:39:PHE:CE2	3:A:46:ARG:CZ	2.97	0.47
2:l:106:ILE:H	2:l:166:GLN:HE22	1.64	0.46
3:A:7:ILE:O	3:A:9:PRO:HD3	2.16	0.46
3:F:39:PHE:CE2	3:F:46:ARG:CZ	2.99	0.45
3:F:7:ILE:O	3:F:9:PRO:HD3	2.18	0.44
1:H:190:THR:HG22	1:H:190:THR:O	2.17	0.44
3:F:4:LEU:HD23	3:F:5:GLN:N	2.33	0.44
3:F:31:ILE:HA	3:F:32:PRO:C	2.44	0.43
1:H:57:GLU:OE1	3:A:95:ARG:NH1	2.48	0.43
3:F:92:VAL:HG22	3:F:106:SER:HB3	2.01	0.42
2:L:33:LEU:HD11	2:L:88:CYS:HB2	2.00	0.42
2:l:183:LYS:O	2:l:184:ALA:C	2.62	0.42
2:l:112:ALA:HB2	2:l:200:GLY:O	2.19	0.42
1:H:152:TYR:CE1	1:H:157:VAL:HG23	2.55	0.42
3:A:4:LEU:HD23	3:A:5:GLN:N	2.35	0.42
3:A:38:TRP:CD1	3:A:76:ILE:HD13	2.55	0.41
3:A:49:ILE:O	3:A:60:VAL:HG21	2.20	0.41
1:H:11:VAL:HG21	1:H:154:PRO:HG3	2.03	0.41
2:L:112:ALA:HB2	2:L:200:GLY:O	2.21	0.41
2:l:33:LEU:HD11	2:l:88:CYS:HB2	2.03	0.41
3:A:34:GLY:HA3	3:A:94:PHE:O	2.21	0.41
3:F:49:ILE:O	3:F:60:VAL:HG21	2.21	0.40
1:h:99:GLU:OE2	1:h:105:TYR:HA	2.22	0.40

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	H	200/227 (88%)	192 (96%)	8 (4%)	0	100	100
1	h	200/227 (88%)	191 (96%)	9 (4%)	0	100	100
2	L	209/214 (98%)	195 (93%)	13 (6%)	1 (0%)	24	27
2	l	209/214 (98%)	195 (93%)	13 (6%)	1 (0%)	24	27
3	A	98/125 (78%)	91 (93%)	7 (7%)	0	100	100
3	F	96/125 (77%)	90 (94%)	6 (6%)	0	100	100
All	All	1012/1132 (89%)	954 (94%)	56 (6%)	2 (0%)	43	51

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	l	204	PRO
2	L	204	PRO

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	H	144/189 (76%)	139 (96%)	5 (4%)	32	43
1	h	133/189 (70%)	129 (97%)	4 (3%)	36	49
2	L	146/184 (79%)	140 (96%)	6 (4%)	27	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	l	128/184 (70%)	121 (94%)	7 (6%)	19	24
3	A	72/104 (69%)	70 (97%)	2 (3%)	38	52
3	F	73/104 (70%)	70 (96%)	3 (4%)	27	37
All	All	696/954 (73%)	669 (96%)	27 (4%)	28	39

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	7	SER
1	H	17	SER
1	H	43	GLN
1	H	88	SER
1	H	190	THR
2	L	30	SER
2	L	89	GLN
2	L	90	GLN
2	L	105	GLU
2	L	107	LYS
2	L	158	ASN
3	F	20	THR
3	F	26	THR
3	F	61	THR
1	h	7	SER
1	h	17	SER
1	h	43	GLN
1	h	206	ASN
2	l	30	SER
2	l	55	GLN
2	l	89	GLN
2	l	90	GLN
2	l	105	GLU
2	l	107	LYS
2	l	158	ASN
3	A	26	THR
3	A	61	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	3	GLN

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Mol	Chain	Res	Type
1	H	39	GLN
1	H	178	GLN
2	L	38	GLN
2	L	55	GLN
2	L	89	GLN
2	L	90	GLN
2	L	138	ASN
2	L	155	GLN
2	L	158	ASN
2	L	160	GLN
2	L	166	GLN
2	L	198	HIS
3	F	37	GLN
3	F	71	ASN
1	h	3	GLN
1	h	39	GLN
1	h	43	GLN
1	h	171	HIS
1	h	178	GLN
2	l	38	GLN
2	l	89	GLN
2	l	90	GLN
2	l	137	ASN
2	l	158	ASN
2	l	160	GLN
2	l	166	GLN
2	l	189	HIS
2	l	198	HIS
3	A	37	GLN
3	A	71	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 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	$\# Z > 2$
4	EDO	l	302	-	3,3,3	0.85	0	2,2,2	0.51	0
4	EDO	H	301	-	3,3,3	0.85	0	2,2,2	0.16	0
5	GOL	L	301	-	5,5,5	0.48	0	5,5,5	0.83	0
4	EDO	l	301	-	3,3,3	0.71	0	2,2,2	0.26	0
4	EDO	l	303	-	3,3,3	0.48	0	2,2,2	0.22	0
4	EDO	F	201	-	3,3,3	0.77	0	2,2,2	0.45	0
4	EDO	A	201	-	3,3,3	0.53	0	2,2,2	0.19	0

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
4	EDO	l	302	-	-	1/1/1/1	-
4	EDO	H	301	-	-	1/1/1/1	-
5	GOL	L	301	-	-	2/4/4/4	-
4	EDO	l	301	-	-	0/1/1/1	-
4	EDO	l	303	-	-	1/1/1/1	-
4	EDO	F	201	-	-	1/1/1/1	-
4	EDO	A	201	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	301	EDO	O1-C1-C2-O2
5	L	301	GOL	O1-C1-C2-C3
4	I	303	EDO	O1-C1-C2-O2
5	L	301	GOL	O1-C1-C2-O2
4	I	302	EDO	O1-C1-C2-O2
4	A	201	EDO	O1-C1-C2-O2
4	F	201	EDO	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, 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	H	206/227 (90%)	0.78	28 (13%) 7 5	16, 37, 74, 82	0
1	h	206/227 (90%)	1.16	48 (23%) 2 1	17, 41, 84, 96	0
2	L	211/214 (98%)	0.81	23 (10%) 10 8	18, 42, 64, 77	0
2	l	211/214 (98%)	1.05	34 (16%) 4 3	18, 44, 65, 77	0
3	A	104/125 (83%)	2.05	49 (47%) 0 0	26, 52, 66, 77	0
3	F	102/125 (81%)	2.13	59 (57%) 0 0	24, 54, 74, 77	0
All	All	1040/1132 (91%)	1.18	241 (23%) 2 1	16, 44, 74, 96	0

All (241) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	112	LEU	7.2
3	A	38	TRP	6.0
1	h	143	ALA	5.6
1	h	200	THR	5.4
3	A	89	TYR	5.4
1	h	191	VAL	5.3
3	F	13	VAL	5.3
3	A	21	ALA	5.3
3	F	89	TYR	5.2
3	F	38	TRP	5.0
3	A	108	ALA	4.9
3	A	23	LEU	4.8
1	h	133	PRO	4.7
1	h	190	THR	4.7
3	A	76	ILE	4.5
1	h	189	VAL	4.4
3	A	88	THR	4.4
3	F	21	ALA	4.4
1	h	212	THR	4.3

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Mol	Chain	Res	Type	RSRZ
3	F	23	LEU	4.3
1	h	218	VAL	4.3
3	F	110	THR	4.3
3	A	107	GLY	4.3
1	H	191	VAL	4.3
3	A	60	VAL	4.2
2	l	201	LEU	4.1
2	L	188	LYS	4.0
3	F	44	PRO	4.0
3	A	90	TYR	4.0
3	A	91	CYS	3.9
1	h	193	SER	3.9
3	A	13	VAL	3.9
3	F	61	THR	3.8
3	A	113	SER	3.8
3	A	112	LEU	3.8
1	h	163	SER	3.7
2	l	109	THR	3.7
1	h	194	SER	3.7
3	A	39	PHE	3.6
1	h	149	VAL	3.6
1	h	11	VAL	3.5
1	h	188	VAL	3.5
3	A	86	ALA	3.5
3	F	56	HIS	3.5
3	F	76	ILE	3.4
3	A	111	GLU	3.4
3	F	86	ALA	3.4
3	F	24	ARG	3.4
1	H	133	PRO	3.4
2	l	14	SER	3.4
3	F	108	ALA	3.4
3	A	42	ALA	3.4
1	h	211	ASN	3.4
3	A	56	HIS	3.3
1	H	189	VAL	3.3
3	A	75	SER	3.3
2	L	185	ASP	3.3
3	A	20	THR	3.3
3	A	110	THR	3.3
2	l	110	VAL	3.3
1	H	145	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
2	L	210	ASN	3.2
3	F	90	TYR	3.2
1	H	202	ILE	3.2
3	A	78	ILE	3.2
1	h	142	THR	3.2
2	l	208	SER	3.2
2	L	110	VAL	3.2
3	A	6	VAL	3.2
3	F	49	ILE	3.2
3	F	25	CYS	3.2
2	l	112	ALA	3.2
1	h	203	CYS	3.1
3	F	42	ALA	3.1
3	F	107	GLY	3.1
3	A	74	PHE	3.1
2	L	152	ASN	3.1
3	F	78	ILE	3.1
1	h	148	LEU	3.1
1	H	212	THR	3.1
3	F	39	PHE	3.1
3	A	41	GLY	3.0
2	l	138	ASN	3.0
3	F	43	GLY	3.0
1	H	143	ALA	3.0
3	A	102	VAL	2.9
3	A	7	ILE	2.9
3	A	82	THR	2.9
2	l	210	ASN	2.9
1	h	156	PRO	2.9
2	l	191	VAL	2.9
1	H	200	THR	2.9
3	A	22	THR	2.9
1	H	220	PRO	2.9
3	F	26	THR	2.9
1	h	215	ASP	2.9
3	F	87	GLY	2.9
1	H	144	ALA	2.9
1	h	166	LEU	2.9
3	F	74	PHE	2.9
3	F	60	VAL	2.9
3	F	82	THR	2.9
1	h	129	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
2	l	202	SER	2.8
3	F	75	SER	2.8
1	h	192	PRO	2.8
3	F	57	PHE	2.8
3	F	22	THR	2.7
3	A	25	CYS	2.7
3	F	50	TYR	2.7
1	h	205	VAL	2.7
3	F	11	LYS	2.7
1	H	157	VAL	2.7
3	A	92	VAL	2.7
2	L	138	ASN	2.7
3	A	44	PRO	2.7
3	F	91	CYS	2.7
2	l	116	PHE	2.7
1	H	218	VAL	2.7
3	F	55	GLY	2.7
3	F	59	ARG	2.7
3	F	84	ALA	2.6
3	F	102	VAL	2.6
3	F	83	PRO	2.6
3	A	24	ARG	2.6
3	A	40	ARG	2.6
3	F	8	GLN	2.6
3	A	11	LYS	2.6
3	A	84	ALA	2.6
2	l	118	PHE	2.6
1	h	131	LEU	2.6
1	h	132	ALA	2.6
2	l	111	ALA	2.6
3	F	77	ARG	2.6
3	F	92	VAL	2.6
1	h	219	GLU	2.6
2	L	194	CYS	2.6
1	h	158	THR	2.6
1	h	220	PRO	2.6
3	A	109	GLY	2.6
1	h	144	ALA	2.5
3	A	10	ASP	2.5
1	h	170	VAL	2.5
2	L	202	SER	2.5
1	H	199	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	206	ASN	2.5
1	h	162	ASN	2.5
2	L	193	ALA	2.5
2	L	163	VAL	2.5
3	F	64	SER	2.5
1	H	142	THR	2.5
1	h	160	SER	2.5
1	h	145	LEU	2.5
3	F	109	GLY	2.5
2	l	9	SER	2.4
1	H	204	ASN	2.4
3	F	85	ASP	2.4
1	h	169	GLY	2.4
2	L	204	PRO	2.4
3	A	87	GLY	2.4
2	l	168	SER	2.4
1	h	202	ILE	2.4
1	h	168	SER	2.4
1	h	210	SER	2.4
2	l	114	SER	2.4
2	L	209	PHE	2.4
2	L	180	THR	2.4
3	F	88	THR	2.4
2	L	208	SER	2.4
1	H	203	CYS	2.4
2	l	115	VAL	2.4
2	l	194	CYS	2.4
1	H	219	GLU	2.4
2	l	148	TRP	2.4
2	l	119	PRO	2.3
1	h	55	GLY	2.3
2	l	129	THR	2.3
3	A	61	THR	2.3
2	L	205	VAL	2.3
2	L	181	LEU	2.3
3	F	9	PRO	2.3
2	l	16	GLY	2.3
1	h	123	THR	2.3
3	A	63	VAL	2.3
1	h	209	PRO	2.3
3	A	83	PRO	2.3
2	l	64	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
3	A	55	GLY	2.3
3	F	48	LEU	2.3
3	A	105	LYS	2.3
3	F	41	GLY	2.3
3	F	6	VAL	2.3
3	F	63	VAL	2.3
1	H	211	ASN	2.2
2	l	193	ALA	2.2
1	h	161	TRP	2.2
3	F	12	SER	2.2
1	H	205	VAL	2.2
2	l	125	LEU	2.2
3	A	12	SER	2.2
2	L	125	LEU	2.2
2	L	136	LEU	2.2
1	H	215	ASP	2.2
1	H	169	GLY	2.2
2	l	189	HIS	2.2
1	H	170	VAL	2.2
2	L	115	VAL	2.2
3	F	94	PHE	2.2
2	l	23	CYS	2.2
2	l	172	THR	2.2
1	h	185	LEU	2.1
2	l	188	LYS	2.1
3	F	19	GLU	2.1
1	h	56	GLY	2.1
2	l	203	SER	2.1
1	H	166	LEU	2.1
2	L	117	ILE	2.1
3	F	36	ILE	2.1
1	H	188	VAL	2.1
3	A	77	ARG	2.1
2	L	203	SER	2.1
2	l	199	GLN	2.1
1	h	157	VAL	2.1
1	H	163	SER	2.1
2	L	111	ALA	2.1
2	l	144	ALA	2.1
2	l	170	ASP	2.1
2	l	150	VAL	2.1
3	A	59	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	h	217	LYS	2.0
1	H	193	SER	2.0
1	h	16	ALA	2.0
1	h	147	CYS	2.0
3	F	73	ASP	2.0
3	F	58	PRO	2.0
1	H	201	TYR	2.0
2	L	19	VAL	2.0
3	F	20	THR	2.0
3	F	47	GLU	2.0
3	F	106	SER	2.0
3	A	2	GLU	2.0

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 oligosaccharides 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. 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
4	EDO	A	201	4/4	0.81	0.19	58,61,61,62	0
4	EDO	H	301	4/4	0.84	0.18	50,52,53,53	0
4	EDO	l	302	4/4	0.88	0.17	33,41,42,43	0
4	EDO	l	301	4/4	0.88	0.14	39,47,52,52	0
4	EDO	l	303	4/4	0.89	0.17	53,59,60,61	0
5	GOL	L	301	6/6	0.92	0.13	44,47,50,51	0
4	EDO	F	201	4/4	0.94	0.09	39,40,42,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.