



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 08:58 PM UTC

PDB ID : 8BE1 / pdb_00008be1
Title : SARS-CoV-2 RBD in complex with a Fab fragment of a neutralising antibody mRBD2
Authors : Lulla, A.; Brear, P.; Fischer, K.; Hollfelder, F.; Hyvonen, M.
Deposited on : 2022-10-21
Resolution : 1.98 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

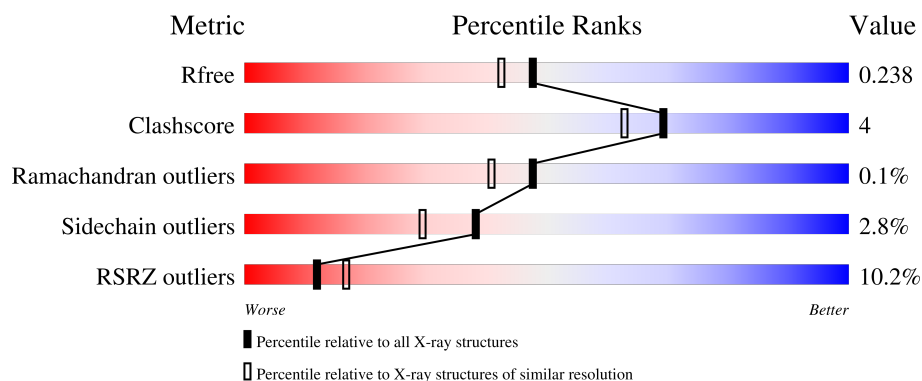
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	A	230	3% 87% 7% 6%
1	D	230	7% 81% 11% 7%
2	B	215	3% 90% 9% .
2	E	215	6% 87% 11% .
3	C	198	24% 82% 8% . 9%

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Mol	Chain	Length	Quality of chain
3	F	198	

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
4	SO4	A	301	-	X	X	-
4	SO4	D	302	-	X	-	-
4	SO4	E	301	-	X	X	-
4	SO4	F	601	-	-	X	-
4	SO4	F	603	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9866 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 Antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1643	1040	271	326	6			
1	D	213	Total	C	N	O	S	0	0	0
			1622	1030	267	318	7			

- Molecule 2 is a protein called Antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	0	0	0
			1659	1032	279	342	6			
2	E	213	Total	C	N	O	S	0	0	0
			1659	1032	279	342	6			

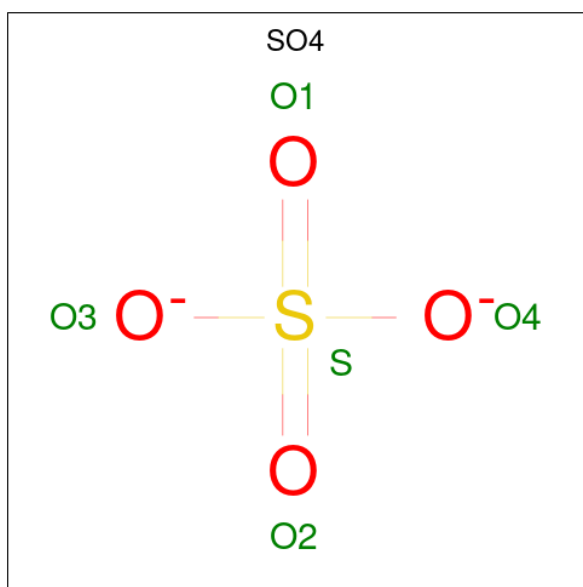
- Molecule 3 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	180	Total	C	N	O	S	0	1	0
			1434	919	239	269	7			
3	F	186	Total	C	N	O	S	0	1	0
			1478	948	245	277	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	330	GLY	-	expression tag	UNP P0DTC2
C	331	SER	-	expression tag	UNP P0DTC2
C	332	GLY	-	expression tag	UNP P0DTC2
F	330	GLY	-	expression tag	UNP P0DTC2
F	331	SER	-	expression tag	UNP P0DTC2
F	332	GLY	-	expression tag	UNP P0DTC2

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		

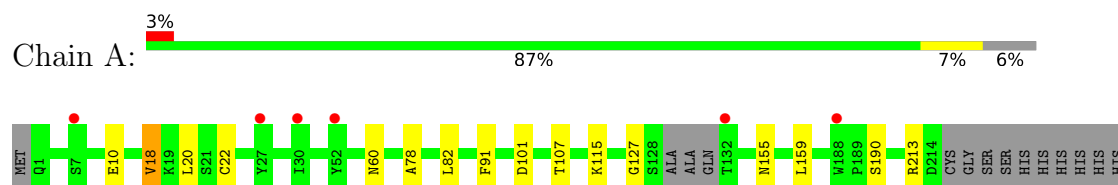
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	62	Total	O	0	0
			62	62		
5	B	68	Total	O	0	0
			68	68		
5	C	26	Total	O	0	0
			26	26		
5	D	49	Total	O	0	0
			49	49		
5	E	44	Total	O	0	0
			44	44		
5	F	37	Total	O	0	0
			37	37		

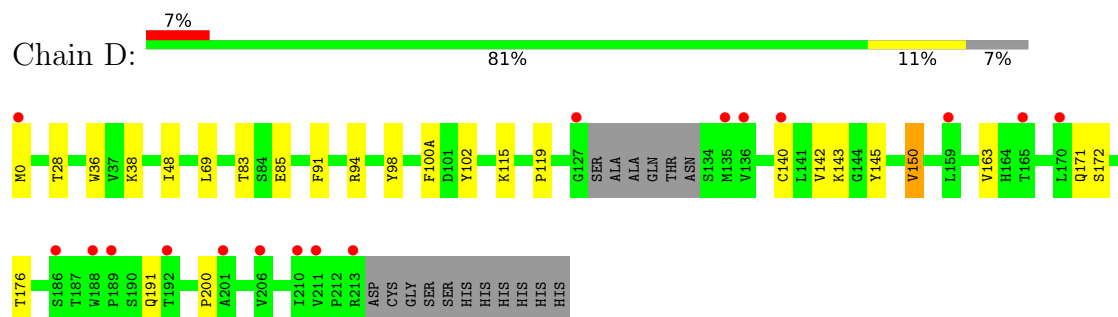
3 Residue-property plots [i](#)

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.

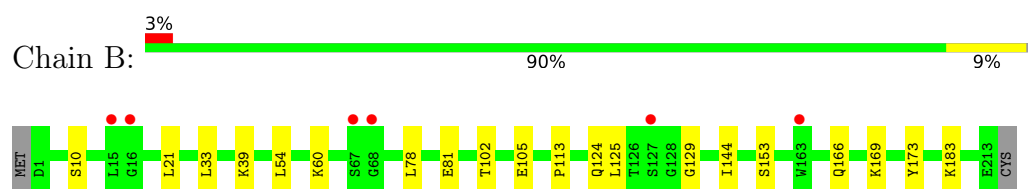
- Molecule 1: Antibody heavy chain



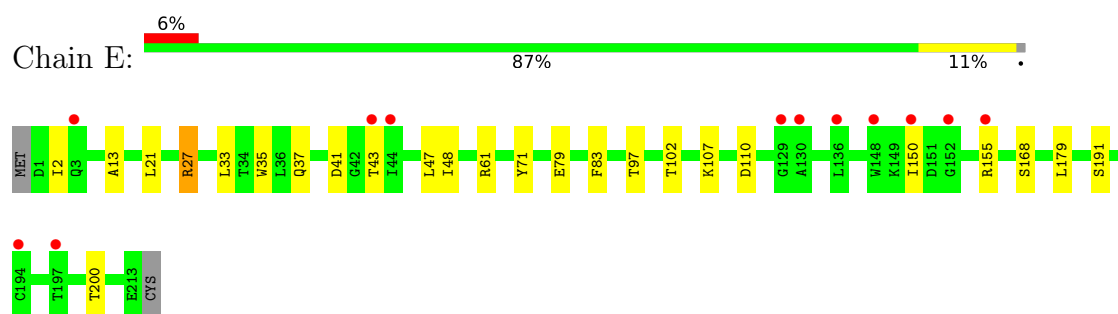
- Molecule 1: Antibody heavy chain



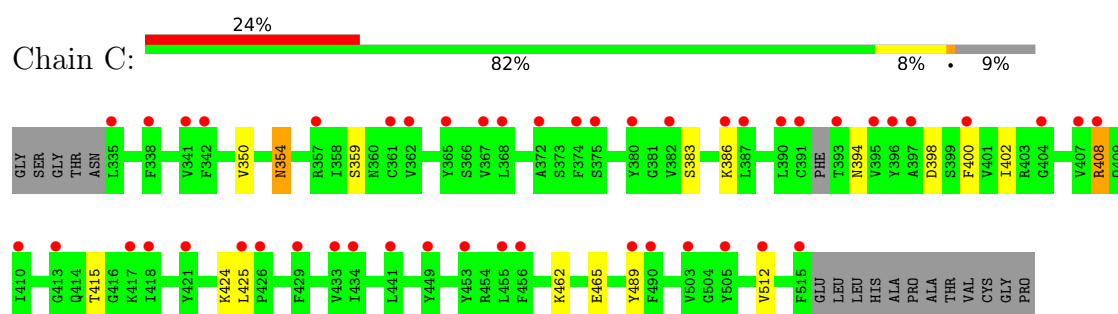
- Molecule 2: Antibody light chain



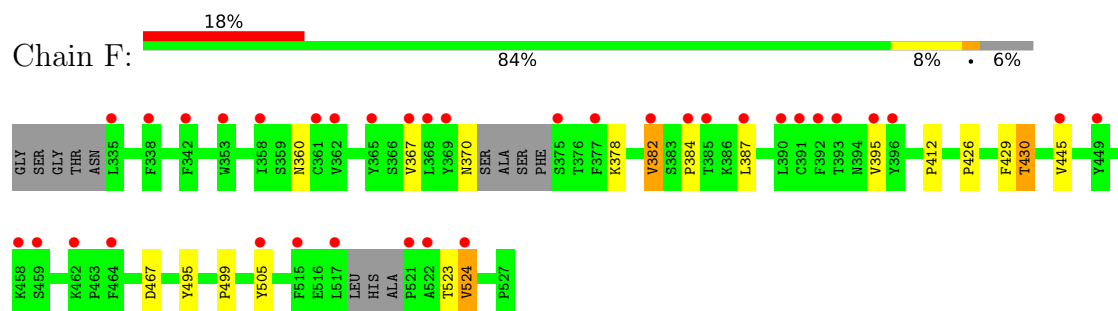
- Molecule 2: Antibody light chain



- Molecule 3: Spike protein S1



• Molecule 3: Spike protein S1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.47Å 194.62Å 62.09Å 90.00° 97.16° 90.00°	Depositor
Resolution (Å)	39.02 – 1.98 39.02 – 1.98	Depositor EDS
% Data completeness (in resolution range)	98.2 (39.02-1.98) 98.2 (39.02-1.98)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 1.98Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.247 , 0.284 0.238 , 0.238	Depositor DCC
R_{free} test set	4659 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	55.7	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9866	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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

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	0.76	0/1685	0.99	4/2298 (0.2%)
1	D	0.74	0/1664	0.98	3/2268 (0.1%)
2	B	0.72	0/1695	0.99	0/2298
2	E	0.74	0/1695	1.00	1/2298 (0.0%)
3	C	0.78	2/1466 (0.1%)	0.96	2/1990 (0.1%)
3	F	0.76	0/1510	1.02	4/2048 (0.2%)
All	All	0.75	2/9715 (0.0%)	0.99	14/13200 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	359	SER	CA-C	14.08	1.59	1.52
3	C	402	ILE	CA-C	5.52	1.57	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	499	PRO	CA-C-N	6.31	129.90	120.31
3	F	499	PRO	C-N-CA	6.31	129.90	120.31
1	A	60	ASN	CA-CB-CG	6.11	118.71	112.60
1	D	28	THR	CA-C-N	6.06	128.68	120.38
1	D	28	THR	C-N-CA	6.06	128.68	120.38
3	F	495	TYR	N-CA-C	-6.00	100.72	110.20
1	A	91	PHE	CA-CB-CG	5.92	119.72	113.80
2	E	83	PHE	CA-CB-CG	-5.74	108.06	113.80
1	A	101	ASP	CA-CB-CG	5.64	118.24	112.60
3	C	489	TYR	N-CA-C	5.18	118.26	109.76
3	C	359	SER	N-CA-C	5.16	116.35	108.30
1	D	91	PHE	CA-CB-CG	5.08	118.88	113.80
1	A	60	ASN	N-CA-C	-5.07	102.35	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	467	ASP	CA-CB-CG	5.04	117.64	112.60

There are no chirality outliers.

There are no planarity outliers.

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	1643	0	1598	5	0
1	D	1622	0	1585	13	0
2	B	1659	0	1591	9	0
2	E	1659	0	1591	13	0
3	C	1434	0	1355	6	0
3	F	1478	0	1398	13	0
4	A	10	0	0	4	0
4	B	10	0	0	0	0
4	C	10	0	0	1	0
4	D	25	0	0	3	0
4	E	15	0	0	6	0
4	F	15	0	0	5	0
5	A	62	0	0	0	0
5	B	68	0	0	0	0
5	C	26	0	0	0	0
5	D	49	0	0	0	0
5	E	44	0	0	0	0
5	F	37	0	0	1	0
All	All	9866	0	9118	66	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 4.

All (66) 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)
4:E:301:SO4:S	4:E:301:SO4:O3	1.03	1.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:301:SO4:O4	4:A:301:SO4:S	1.01	1.41
4:E:301:SO4:O3	4:E:301:SO4:O2	1.65	1.12
4:A:301:SO4:O4	4:A:301:SO4:O3	1.69	1.08
4:A:301:SO4:O4	4:A:301:SO4:O2	1.74	1.02
4:A:301:SO4:O4	4:A:301:SO4:O1	1.78	1.00
4:E:301:SO4:O3	4:E:301:SO4:O1	1.84	0.96
4:E:301:SO4:O3	4:E:301:SO4:O4	1.83	0.95
1:D:119:PRO:HB3	1:D:145:TYR:HB3	1.67	0.76
2:B:39:LYS:HZ1	2:B:81:GLU:HG2	1.56	0.68
2:E:150:ILE:HD12	2:E:155:ARG:HD2	1.79	0.65
2:E:155:ARG:HG3	4:E:302:SO4:O1	1.98	0.64
2:B:39:LYS:NZ	2:B:81:GLU:HG2	2.12	0.63
3:C:408:ARG:NH2	4:C:601:SO4:O4	2.32	0.62
3:F:505:TYR:HD2	4:F:602:SO4:O4	1.85	0.59
3:F:430:THR:O	4:F:603:SO4:O3	2.22	0.57
2:E:61:ARG:CZ	2:E:79:GLU:HG3	2.35	0.57
3:F:429:PHE:HD1	4:F:603:SO4:O4	1.87	0.57
2:B:21:LEU:HD22	2:B:102:THR:HG21	1.86	0.57
3:F:395:VAL:HG23	3:F:524:VAL:HG11	1.86	0.56
3:C:462:LYS:HG2	3:C:465:GLU:HB2	1.87	0.56
1:A:18:VAL:HG12	1:A:82:LEU:HB2	1.89	0.55
3:C:383:SER:HB3	3:C:386:LYS:HG2	1.90	0.54
2:E:13:ALA:HA	2:E:107:LYS:HE3	1.90	0.54
1:D:143:LYS:HE3	1:D:176:THR:HG21	1.91	0.51
1:D:143:LYS:HE2	1:D:171:GLN:OE1	2.11	0.51
2:E:150:ILE:HD11	2:E:179:LEU:HD21	1.92	0.51
2:E:97:THR:HA	4:E:301:SO4:O1	2.12	0.49
2:E:33:LEU:HD22	2:E:71:TYR:HB3	1.95	0.49
3:F:505:TYR:CD1	4:F:601:SO4:O4	2.67	0.48
1:D:142:VAL:HG11	1:D:150:VAL:HG11	1.96	0.47
3:F:412:PRO:HG3	3:F:429:PHE:HB3	1.96	0.47
1:D:83:THR:HG23	1:D:85:GLU:H	1.80	0.46
1:D:36:TRP:CD1	1:D:69:LEU:HD22	2.50	0.46
2:E:37:GLN:HB2	2:E:47:LEU:HD11	1.99	0.45
3:F:360:ASN:H	3:F:523:THR:HB	1.82	0.45
3:F:412:PRO:HB3	3:F:426:PRO:O	2.17	0.45
1:D:38:LYS:HB2	1:D:48:ILE:HD11	1.99	0.45
1:A:155:ASN:HB2	1:A:159:LEU:HG	1.99	0.45
1:D:163:VAL:HG21	4:D:304:SO4:O3	2.17	0.44
1:D:98:TYR:CD2	4:D:303:SO4:O4	2.70	0.44
2:E:110:ASP:HB3	2:E:200:THR:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:384:PRO:HA	3:F:387:LEU:HD12	1.99	0.43
1:A:20:LEU:HD22	1:A:107:THR:HG21	2.00	0.43
1:D:119:PRO:CB	1:D:145:TYR:HB3	2.44	0.43
3:F:505:TYR:CE1	4:F:601:SO4:O4	2.72	0.42
3:C:354:ASN:O	3:C:398:ASP:HA	2.19	0.42
1:A:22:CYS:HB3	1:A:78:ALA:HB3	2.01	0.42
2:B:166:GLN:HG3	2:B:173:TYR:CZ	2.53	0.42
2:E:35:TRP:HB2	2:E:48:ILE:HB	2.02	0.42
3:F:360:ASN:H	3:F:523:THR:CB	2.33	0.42
3:F:378:LYS:NZ	5:F:705:HOH:O	2.52	0.42
1:A:127:GLY:HA2	1:A:213:ARG:HD2	2.01	0.42
2:B:125:LEU:O	2:B:183:LYS:HD2	2.20	0.41
2:E:2:ILE:HG12	2:E:27:ARG:HG3	2.02	0.41
3:F:382:VAL:HG23	3:F:387:LEU:HG	2.02	0.41
2:B:39:LYS:NZ	2:B:81:GLU:CG	2.83	0.41
2:B:169:LYS:HB2	1:D:102:TYR:CE2	2.55	0.41
2:E:21:LEU:HD22	2:E:102:THR:HG21	2.03	0.41
2:B:113:PRO:HG3	2:B:144:ILE:HD11	2.03	0.41
3:C:425:LEU:HD21	3:C:512:VAL:HG11	2.01	0.41
1:D:200:PRO:HA	4:D:305:SO4:O3	2.21	0.41
1:D:94:ARG:O	1:D:100(A):PHE:HA	2.20	0.41
2:E:41:ASP:OD1	2:E:43:THR:HG22	2.21	0.41
2:B:124:GLN:HG2	2:B:129:GLY:O	2.21	0.41
3:C:350:VAL:HA	3:C:400:PHE:HB2	2.03	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	A	212/230 (92%)	209 (99%)	3 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	209/230 (91%)	205 (98%)	3 (1%)	1 (0%)	24	14
2	B	211/215 (98%)	206 (98%)	5 (2%)	0	100	100
2	E	211/215 (98%)	206 (98%)	5 (2%)	0	100	100
3	C	176/198 (89%)	164 (93%)	12 (7%)	0	100	100
3	F	180/198 (91%)	172 (96%)	8 (4%)	0	100	100
All	All	1199/1286 (93%)	1162 (97%)	36 (3%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	172	SER

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	185/196 (94%)	181 (98%)	4 (2%)	45	38
1	D	182/196 (93%)	177 (97%)	5 (3%)	39	31
2	B	189/191 (99%)	182 (96%)	7 (4%)	30	20
2	E	189/191 (99%)	186 (98%)	3 (2%)	55	50
3	C	155/169 (92%)	150 (97%)	5 (3%)	34	24
3	F	160/169 (95%)	154 (96%)	6 (4%)	29	19
All	All	1060/1112 (95%)	1030 (97%)	30 (3%)	38	29

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLU
1	A	18	VAL
1	A	115	LYS
1	A	190	SER
2	B	10	SER

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Mol	Chain	Res	Type
2	B	33	LEU
2	B	54	LEU
2	B	60	LYS
2	B	78	LEU
2	B	105	GLU
2	B	153	SER
3	C	354	ASN
3	C	394	ASN
3	C	408	ARG
3	C	415	THR
3	C	424	LYS
1	D	0	MET
1	D	115	LYS
1	D	140	CYS
1	D	150	VAL
1	D	191	GLN
2	E	27	ARG
2	E	168	SER
2	E	191	SER
3	F	367	VAL
3	F	370	ASN
3	F	382	VAL
3	F	430	THR
3	F	445	VAL
3	F	524	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	32	ASN
3	C	360	ASN
2	E	190	ASN
3	F	360	ASN
3	F	394	ASN
3	F	439	ASN
3	F	450	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

17 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	SO4	A	301	-	4,4,4	4.53	4 (100%)	6,6,6	0.97	0
4	SO4	E	302	-	4,4,4	1.84	1 (25%)	6,6,6	1.24	1 (16%)
4	SO4	F	601	-	4,4,4	2.12	1 (25%)	6,6,6	0.91	0
4	SO4	B	302	-	4,4,4	0.32	0	6,6,6	0.30	0
4	SO4	B	301	-	4,4,4	1.08	0	6,6,6	0.96	0
4	SO4	D	304	-	4,4,4	0.68	0	6,6,6	0.78	0
4	SO4	D	305	-	4,4,4	0.36	0	6,6,6	0.32	0
4	SO4	D	301	-	4,4,4	0.34	0	6,6,6	0.48	0
4	SO4	C	601	-	4,4,4	0.22	0	6,6,6	0.17	0
4	SO4	F	602	-	4,4,4	0.37	0	6,6,6	0.32	0
4	SO4	C	602	-	4,4,4	0.26	0	6,6,6	0.20	0
4	SO4	D	302	-	4,4,4	2.94	3 (75%)	6,6,6	1.66	2 (33%)
4	SO4	E	303	-	4,4,4	0.40	0	6,6,6	0.19	0
4	SO4	A	302	-	4,4,4	0.58	0	6,6,6	0.56	0
4	SO4	D	303	-	4,4,4	1.35	1 (25%)	6,6,6	0.74	0
4	SO4	F	603	-	4,4,4	0.45	0	6,6,6	0.53	0
4	SO4	E	301	-	4,4,4	4.45	4 (100%)	6,6,6	1.24	1 (16%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	301	SO4	O4-S	-5.64	1.01	1.48
4	E	301	SO4	O3-S	-5.40	1.03	1.48
4	E	301	SO4	O2-S	-4.83	1.16	1.44
4	A	301	SO4	O2-S	-4.53	1.18	1.44
4	D	302	SO4	O4-S	-4.19	1.13	1.48
4	A	301	SO4	O3-S	-4.17	1.13	1.48
4	E	301	SO4	O1-S	-3.95	1.21	1.44
4	A	301	SO4	O1-S	-3.52	1.24	1.44
4	E	301	SO4	O4-S	-3.31	1.21	1.48
4	D	302	SO4	O1-S	-3.16	1.26	1.44
4	F	601	SO4	O2-S	-3.03	1.27	1.44
4	D	302	SO4	O3-S	-2.26	1.29	1.48
4	E	302	SO4	O1-S	-2.13	1.32	1.44
4	D	303	SO4	O2-S	-2.02	1.33	1.44

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	302	SO4	O4-S-O1	-2.63	95.81	109.56
4	E	302	SO4	O4-S-O1	-2.35	97.29	109.56
4	E	301	SO4	O3-S-O2	-2.33	97.38	109.56
4	D	302	SO4	O3-S-O2	2.08	120.45	109.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	301	SO4	4	0
4	E	302	SO4	1	0
4	F	601	SO4	2	0
4	D	304	SO4	1	0
4	D	305	SO4	1	0
4	C	601	SO4	1	0
4	F	602	SO4	1	0
4	D	303	SO4	1	0
4	F	603	SO4	2	0
4	E	301	SO4	5	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

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	216/230 (93%)	0.77	6 (2%) 55 65	46, 60, 78, 87	0
1	D	213/230 (92%)	0.98	17 (7%) 18 25	44, 66, 83, 93	0
2	B	213/215 (99%)	0.63	6 (2%) 55 65	47, 58, 72, 86	0
2	E	213/215 (99%)	0.82	12 (5%) 30 38	40, 63, 79, 105	0
3	C	180/198 (90%)	1.48	48 (26%) 1 1	57, 74, 110, 120	0
3	F	186/198 (93%)	1.17	35 (18%) 3 4	44, 63, 95, 111	0
All	All	1221/1286 (94%)	0.96	124 (10%) 12 17	40, 63, 91, 120	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	456	PHE	4.6
3	F	392	PHE	3.7
3	C	367	VAL	3.7
1	D	0	MET	3.6
3	C	362	VAL	3.4
3	C	515	PHE	3.4
3	F	387	LEU	3.4
3	F	524	VAL	3.4
3	C	393	THR	3.3
3	C	391	CYS	3.3
3	C	335	LEU	3.3
3	C	390	LEU	3.3
3	C	425	LEU	3.3
3	F	368	LEU	3.2
3	C	421	TYR	3.2
3	C	395	VAL	3.1
3	C	338	PHE	3.1
3	C	341	VAL	3.1
2	B	163	TRP	3.1

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Mol	Chain	Res	Type	RSRZ
3	F	382	VAL	3.1
3	F	445	VAL	3.1
3	C	455	LEU	3.0
3	F	395	VAL	3.0
2	B	15	LEU	2.9
3	C	357	ARG	2.9
3	C	396	TYR	2.9
3	F	365	TYR	2.9
2	E	43	THR	2.9
1	D	189	PRO	2.9
3	F	342	PHE	2.9
3	F	515	PHE	2.9
3	F	505	TYR	2.8
3	C	429	PHE	2.8
1	A	30	ILE	2.8
2	E	197	THR	2.8
3	F	335	LEU	2.8
3	C	382	VAL	2.8
3	F	362	VAL	2.8
3	C	397	ALA	2.7
1	D	186	SER	2.7
3	C	512	VAL	2.7
2	E	194	CYS	2.6
1	D	192	THR	2.6
3	C	410	ILE	2.6
3	F	358	ILE	2.6
3	C	380	TYR	2.6
3	C	489	TYR	2.6
3	C	361	CYS	2.6
3	F	517	LEU	2.6
3	C	365	TYR	2.6
3	F	393	THR	2.5
1	D	159	LEU	2.5
2	B	16	GLY	2.5
3	C	404	GLY	2.5
3	C	386	LYS	2.5
3	F	361	CYS	2.5
3	C	503	VAL	2.5
3	F	367	VAL	2.5
1	A	7	SER	2.4
3	C	418	ILE	2.4
1	D	188	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	206	VAL	2.4
3	F	396	TYR	2.4
2	B	67	SER	2.4
1	D	170	LEU	2.4
3	C	441	LEU	2.4
3	C	449	TYR	2.4
3	F	522	ALA	2.4
1	D	127	GLY	2.4
3	C	505	TYR	2.3
3	C	372	ALA	2.3
3	C	413	GLY	2.3
3	F	375	SER	2.3
1	D	140	CYS	2.3
3	F	338	PHE	2.3
3	F	464	PHE	2.3
2	E	44	ILE	2.3
3	F	458	LYS	2.3
3	F	462	LYS	2.3
3	C	387	LEU	2.3
1	A	132	THR	2.3
2	E	152	GLY	2.3
3	C	368	LEU	2.3
3	F	390	LEU	2.3
2	B	68	GLY	2.2
3	C	453	TYR	2.2
2	E	150	ILE	2.2
1	D	211	VAL	2.2
3	C	407	VAL	2.2
2	E	148	TRP	2.2
3	C	490	PHE	2.2
3	F	449	TYR	2.2
1	A	27	TYR	2.2
1	A	52	TYR	2.2
3	F	369	TYR	2.2
3	C	434	ILE	2.2
1	D	135	MET	2.2
1	D	201	ALA	2.2
2	E	130	ALA	2.2
3	C	342	PHE	2.1
3	C	374	PHE	2.1
1	A	188	TRP	2.1
1	D	136	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	127	SER	2.1
3	C	375	SER	2.1
2	E	129	GLY	2.1
1	D	213	ARG	2.1
2	E	155	ARG	2.1
3	C	426	PRO	2.1
1	D	210	ILE	2.1
1	D	165	THR	2.1
3	F	353	TRP	2.1
3	F	385	THR	2.1
3	C	408	ARG	2.1
3	C	433	VAL	2.1
2	E	136	LEU	2.1
2	E	3	GLN	2.1
3	C	417	LYS	2.0
3	F	377	PHE	2.0
3	F	459	SER	2.0
3	F	384	PRO	2.0
3	F	391	CYS	2.0
3	C	400	PHE	2.0
3	F	521	PRO	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($\text{\AA}^2$)	Q<0.9
4	SO4	C	602	5/5	0.71	0.12	102,102,102,103	0
4	SO4	C	601	5/5	0.78	0.12	120,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	D	305	5/5	0.80	0.12	96,96,97,97	0
4	SO4	F	603	5/5	0.80	0.12	81,81,82,82	0
4	SO4	F	602	5/5	0.81	0.16	96,96,97,97	0
4	SO4	E	303	5/5	0.81	0.10	84,84,84,84	0
4	SO4	B	302	5/5	0.87	0.10	83,83,83,83	0
4	SO4	D	301	5/5	0.89	0.10	64,64,65,66	0
4	SO4	A	302	5/5	0.91	0.10	62,62,64,64	0
4	SO4	D	304	5/5	0.93	0.10	63,63,64,65	0
4	SO4	D	303	5/5	0.94	0.09	49,50,53,53	0
4	SO4	D	302	5/5	0.95	0.10	37,40,41,42	0
4	SO4	F	601	5/5	0.95	0.14	44,46,46,49	0
4	SO4	B	301	5/5	0.95	0.11	51,51,55,55	0
4	SO4	E	302	5/5	0.95	0.11	47,47,50,51	0
4	SO4	E	301	5/5	0.98	0.06	31,32,37,37	0
4	SO4	A	301	5/5	0.98	0.07	31,31,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.