



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:26 PM UTC

PDB ID : 7PR0 / pdb_00007pr0
Title : Crystal structure of the receptor binding domain of SARS-CoV-2 Spike glycoprotein in complex with FD-5D Fab
Authors : Zhou, D.; Ren, J.; Stuart, D.I.
Deposited on : 2021-09-20
Resolution : 2.92 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

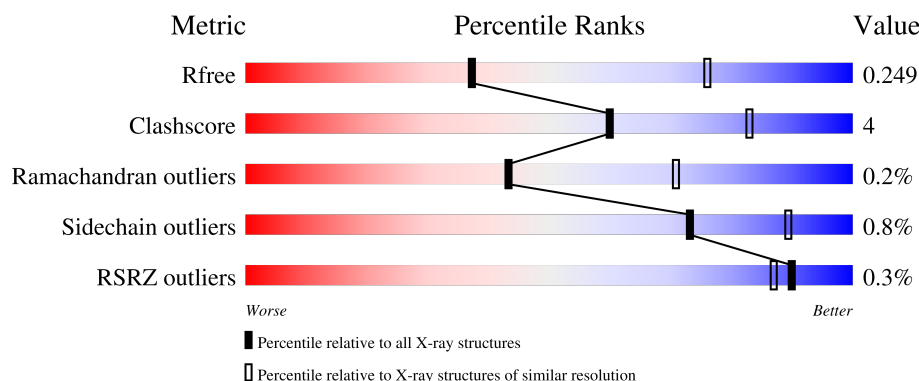
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.92 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	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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	205	
1	D	205	
1	E	205	
2	B	221	
2	F	221	

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Mol	Chain	Length	Quality of chain
2	L	221	90% 10%
3	C	234	85% 10% 5%
3	G	234	66% 15% • 18%
3	H	234	88% 9% •

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14592 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 Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	197	Total	C	N	O	S	0	0	0
			1567	1003	265	291	8			
1	A	199	Total	C	N	O	S	0	0	0
			1581	1011	269	293	8			
1	D	197	Total	C	N	O	S	0	0	0
			1567	1003	265	291	8			

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	324	GLU	-	expression tag	UNP P0DTC2
E	325	THR	-	expression tag	UNP P0DTC2
E	326	GLY	-	expression tag	UNP P0DTC2
E	327	HIS	-	expression tag	UNP P0DTC2
E	328	HIS	-	expression tag	UNP P0DTC2
E	329	HIS	-	expression tag	UNP P0DTC2
E	330	HIS	-	expression tag	UNP P0DTC2
E	331	HIS	-	expression tag	UNP P0DTC2
E	332	HIS	-	expression tag	UNP P0DTC2
E	527	LYS	-	expression tag	UNP P0DTC2
E	528	LYS	-	expression tag	UNP P0DTC2
A	324	GLU	-	expression tag	UNP P0DTC2
A	325	THR	-	expression tag	UNP P0DTC2
A	326	GLY	-	expression tag	UNP P0DTC2
A	327	HIS	-	expression tag	UNP P0DTC2
A	328	HIS	-	expression tag	UNP P0DTC2
A	329	HIS	-	expression tag	UNP P0DTC2
A	330	HIS	-	expression tag	UNP P0DTC2
A	331	HIS	-	expression tag	UNP P0DTC2
A	332	HIS	-	expression tag	UNP P0DTC2
A	527	LYS	-	expression tag	UNP P0DTC2
A	528	LYS	-	expression tag	UNP P0DTC2
D	324	GLU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	325	THR	-	expression tag	UNP P0DTC2
D	326	GLY	-	expression tag	UNP P0DTC2
D	327	HIS	-	expression tag	UNP P0DTC2
D	328	HIS	-	expression tag	UNP P0DTC2
D	329	HIS	-	expression tag	UNP P0DTC2
D	330	HIS	-	expression tag	UNP P0DTC2
D	331	HIS	-	expression tag	UNP P0DTC2
D	332	HIS	-	expression tag	UNP P0DTC2
D	527	LYS	-	expression tag	UNP P0DTC2
D	528	LYS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called FD-5D Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	221	Total	C	N	O	S	0	0	0
			1699	1065	285	342	7			
2	B	219	Total	C	N	O	S	0	0	0
			1684	1057	283	338	6			
2	F	217	Total	C	N	O	S	0	0	0
			1669	1049	278	336	6			

- Molecule 3 is a protein called FD-5D Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	228	Total	C	N	O	S	0	0	0
			1676	1056	278	335	7			
3	C	223	Total	C	N	O	S	0	0	0
			1644	1038	272	327	7			
3	G	191	Total	C	N	O	S	0	0	0
			1421	898	234	282	7			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



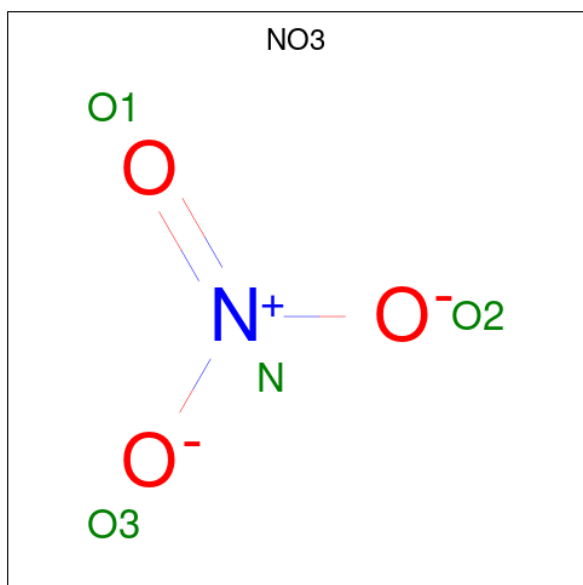
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	1	Total	O S	0	0
			5	4 1		

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

- Molecule 6 is NITRATE ION (CCD ID: NO3) (formula: NO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	N	O	0	0
			4	1	3		
6	H	1	Total	N	O	0	0
			4	1	3		
6	C	1	Total	N	O	0	0
			4	1	3		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	L	1	Total	Cl	0	0
			1	1		
7	H	1	Total	Cl	0	0
			1	1		
7	G	1	Total	Cl	0	0
			1	1		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).

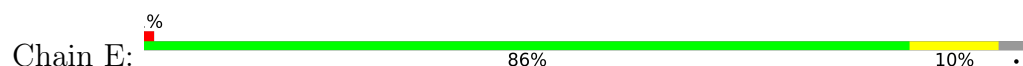


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			6	3	3		
8	F	1	Total	C	O	0	0
			6	3	3		

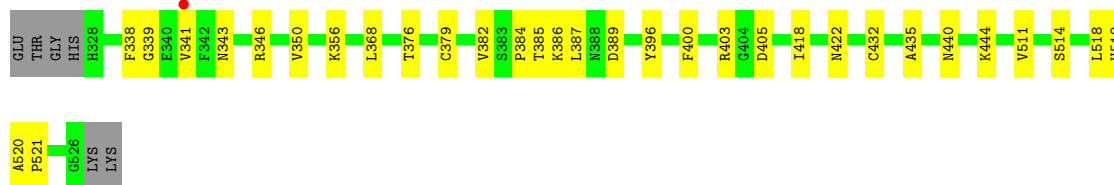
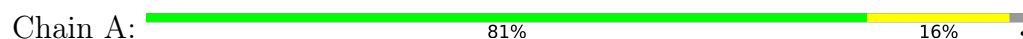
3 Residue-property plots

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: Spike protein S1



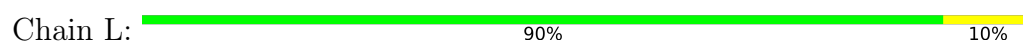
- Molecule 1: Spike protein S1



- Molecule 1: Spike protein S1



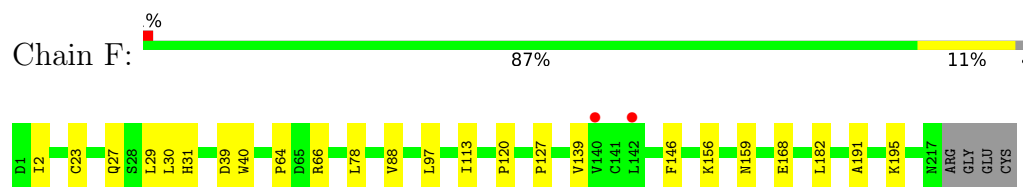
- Molecule 2: FD-5D Fab light chain



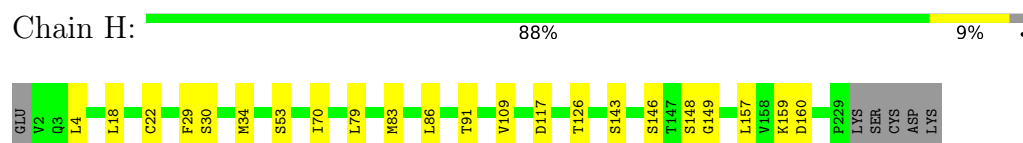
- Molecule 2: FD-5D Fab light chain



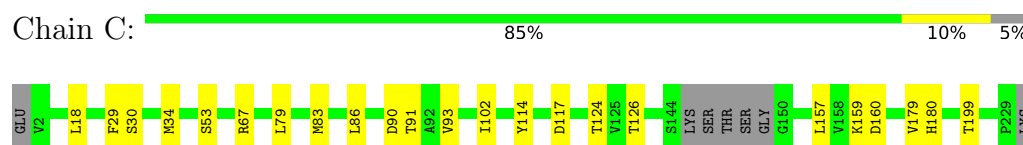
- Molecule 2: FD-5D Fab light chain



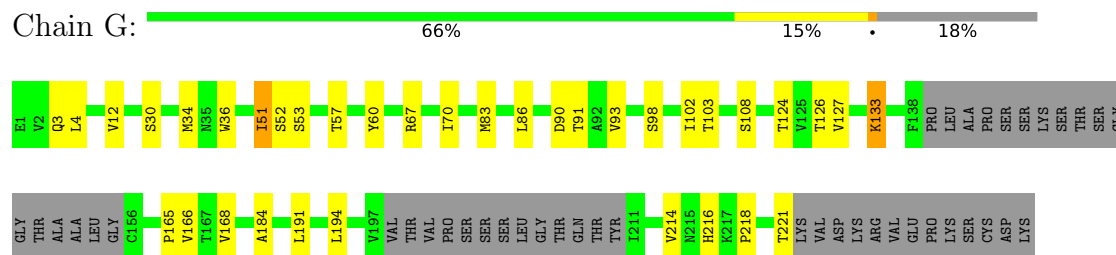
- Molecule 3: FD-5D Fab heavy chain



- Molecule 3: FD-5D Fab heavy chain



- Molecule 3: FD-5D Fab heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	231.31Å 146.06Å 78.58Å 90.00° 103.68° 90.00°	Depositor
Resolution (Å)	71.50 – 2.92 71.50 – 2.92	Depositor EDS
% Data completeness (in resolution range)	92.5 (71.50-2.92) 92.6 (71.50-2.92)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.214 , 0.251 0.214 , 0.249	Depositor DCC
R_{free} test set	2707 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	104.8	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 99.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14592	wwPDB-VP
Average B, all atoms (Å ²)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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, NO3, CL, NAG, 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	0.15	0/1628	0.34	0/2216
1	D	0.14	0/1613	0.35	0/2196
1	E	0.17	0/1613	0.37	0/2196
2	B	0.16	0/1722	0.38	0/2342
2	F	0.16	0/1707	0.36	0/2323
2	L	0.17	0/1737	0.37	0/2362
3	C	0.15	0/1683	0.35	0/2295
3	G	0.16	0/1454	0.35	0/1978
3	H	0.14	0/1716	0.36	0/2340
All	All	0.16	0/14873	0.36	0/20248

There are no bond length outliers.

There are no bond angle outliers.

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	1581	0	1482	20	0
1	D	1567	0	1472	10	0
1	E	1567	0	1472	13	0
2	B	1684	0	1642	16	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1669	0	1626	13	0
2	L	1699	0	1653	13	1
3	C	1644	0	1599	13	0
3	G	1421	0	1367	21	0
3	H	1676	0	1633	14	0
4	A	14	0	13	0	0
4	D	14	0	13	0	0
4	E	14	0	13	0	0
5	E	5	0	0	0	0
5	H	5	0	0	0	0
5	L	5	0	0	0	0
6	C	4	0	0	0	0
6	H	4	0	0	0	0
6	L	4	0	0	0	0
7	G	1	0	0	0	0
7	H	1	0	0	0	0
7	L	1	0	0	0	0
8	B	6	0	8	0	0
8	F	6	0	8	0	0
All	All	14592	0	14001	124	1

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 (124) 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:A:418:ILE:HA	1:A:422:ASN:HD22	1.58	0.69
3:G:52:SER:HB2	3:G:103:THR:HG21	1.76	0.67
2:L:168:GLU:HB2	2:L:182:LEU:HD11	1.75	0.67
3:C:179:VAL:O	3:C:180:HIS:ND1	2.28	0.66
3:G:93:VAL:HG22	3:G:124:THR:HG22	1.77	0.66
1:E:418:ILE:HA	1:E:422:ASN:HD22	1.60	0.66
2:B:168:GLU:HB2	2:B:182:LEU:HD11	1.78	0.66
3:H:143:SER:H	3:H:146:SER:HB3	1.61	0.65
1:E:403:ARG:NH2	1:E:405:ASP:OD2	2.30	0.65
3:G:57:THR:HG21	3:G:108:SER:HB3	1.81	0.61
3:G:67:ARG:NH2	3:G:90:ASP:OD2	2.34	0.60
3:C:93:VAL:HG22	3:C:124:THR:HG22	1.83	0.60
3:H:30:SER:O	3:H:53:SER:OG	2.20	0.60
3:G:83:MET:HB3	3:G:86:LEU:HD21	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:TYR:HD2	2:B:97:LEU:HA	1.66	0.59
1:E:346:ARG:NH2	3:H:117:ASP:OD1	2.35	0.58
2:B:66:ARG:NH1	2:B:87:ASP:OD2	2.35	0.57
2:F:29:LEU:HA	2:F:97:LEU:HD22	1.87	0.56
3:H:148:SER:OG	3:H:149:GLY:N	2.39	0.56
2:L:129:ASP:HA	2:L:132:LEU:HB2	1.87	0.56
1:D:418:ILE:HA	1:D:422:ASN:HD22	1.71	0.55
3:H:34:MET:HB3	3:H:79:LEU:HD22	1.87	0.55
1:E:445:VAL:HG21	2:L:58:ASN:CG	2.32	0.55
3:H:91:THR:HG23	3:H:126:THR:HA	1.88	0.55
3:G:83:MET:HE2	3:G:86:LEU:HD21	1.89	0.54
1:A:389:ASP:HA	1:D:521:PRO:HG3	1.90	0.53
3:C:157:LEU:HD22	3:C:159:LYS:HB2	1.91	0.53
2:F:120:PRO:HB3	2:F:146:PHE:HB3	1.90	0.53
2:F:191:ALA:O	2:F:195:LYS:HG2	2.09	0.52
2:F:156:LYS:HB3	2:F:159:ASN:HA	1.90	0.52
3:G:4:LEU:HD21	3:G:34:MET:HE1	1.92	0.52
2:F:168:GLU:HB2	2:F:182:LEU:HD11	1.91	0.52
1:E:384:PRO:HA	1:E:387:LEU:HG	1.92	0.52
3:H:157:LEU:HD22	3:H:159:LYS:HB2	1.91	0.52
3:C:34:MET:HB3	3:C:79:LEU:HD22	1.91	0.52
1:A:518:LEU:HD12	1:A:520:ALA:HB2	1.92	0.51
1:D:434:ILE:HB	1:D:511:VAL:HG22	1.93	0.51
3:G:91:THR:HG23	3:G:126:THR:HA	1.92	0.51
2:B:88:VAL:HG21	2:B:113:ILE:HD11	1.93	0.51
2:L:196:HIS:O	2:L:218:ARG:HD2	2.11	0.50
1:A:376:THR:HB	1:A:435:ALA:HB3	1.93	0.50
1:A:341:VAL:HG22	1:A:356:LYS:HD2	1.94	0.50
2:B:3:VAL:HG12	2:B:26:SER:HB3	1.93	0.50
2:F:64:PRO:HG2	2:F:66:ARG:HH21	1.77	0.50
3:G:166:VAL:HG12	3:G:216:HIS:HD2	1.76	0.50
1:A:384:PRO:HA	1:A:387:LEU:HG	1.94	0.49
1:A:403:ARG:HE	1:A:405:ASP:HB2	1.76	0.49
3:G:3:GLN:O	3:G:4:LEU:HD12	2.12	0.49
2:B:88:VAL:HG13	2:B:111:VAL:O	2.12	0.49
1:A:403:ARG:NH2	1:A:405:ASP:OD2	2.26	0.49
3:G:216:HIS:CE1	3:G:218:PRO:HG2	2.47	0.49
1:E:392:PHE:HB2	1:A:519:HIS:HB2	1.95	0.48
3:G:30:SER:O	3:G:53:SER:OG	2.32	0.48
3:G:168:VAL:HG23	3:G:214:VAL:HG22	1.96	0.48
2:L:42:LEU:HD13	2:L:91:TYR:CZ	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:30:SER:O	3:C:53:SER:OG	2.32	0.47
2:F:40:TRP:CD2	2:F:78:LEU:HG	2.49	0.47
2:L:220:GLU:HG2	2:L:221:CYS:H	1.79	0.47
2:B:59:ARG:NH1	2:B:65:ASP:HA	2.30	0.47
2:B:149:ARG:HB2	2:B:180:TYR:CE2	2.49	0.47
2:B:23:CYS:HB2	2:B:40:TRP:CH2	2.50	0.46
3:G:36:TRP:HD1	3:G:70:ILE:HD12	1.81	0.46
2:L:194:GLU:HG2	2:L:218:ARG:NH2	2.30	0.46
3:H:70:ILE:HD11	3:H:79:LEU:HD11	1.96	0.46
1:D:379:CYS:HA	1:D:432:CYS:HA	1.98	0.46
3:G:60:TYR:CE1	3:G:70:ILE:HG22	2.51	0.46
3:C:91:THR:HG23	3:C:126:THR:HA	1.98	0.46
1:A:396:TYR:HB2	1:A:514:SER:HB2	1.98	0.46
2:B:191:ALA:O	2:B:195:LYS:HG2	2.16	0.46
3:C:83:MET:HE2	3:C:86:LEU:HD21	1.98	0.46
3:G:133:LYS:HD3	3:G:191:LEU:HD21	1.98	0.46
1:A:440:ASN:OD1	1:A:440:ASN:N	2.49	0.46
1:E:389:ASP:HA	1:A:521:PRO:HG3	1.96	0.45
2:L:194:GLU:HG2	2:L:218:ARG:HH21	1.81	0.45
3:G:51:ILE:HG22	3:G:52:SER:O	2.17	0.45
3:H:29:PHE:CE1	3:H:34:MET:HE3	2.51	0.45
1:A:339:GLY:O	1:A:343:ASN:HB2	2.17	0.45
3:H:83:MET:HB3	3:H:86:LEU:HD21	1.98	0.45
2:B:127:PRO:HB2	2:B:132:LEU:HG	1.99	0.45
1:A:346:ARG:NH2	3:C:117:ASP:OD1	2.49	0.45
1:E:371:SER:C	1:E:373:SER:H	2.25	0.45
1:E:440:ASN:OD1	1:E:440:ASN:N	2.50	0.45
1:E:518:LEU:HD13	1:A:518:LEU:HD21	1.98	0.45
2:F:88:VAL:HG21	2:F:113:ILE:HD11	1.99	0.44
3:G:34:MET:SD	3:G:98:SER:HB2	2.57	0.44
2:B:42:LEU:HD13	2:B:91:TYR:CZ	2.52	0.44
1:E:350:VAL:HA	1:E:400:PHE:HB2	1.99	0.44
1:A:379:CYS:HA	1:A:432:CYS:HA	2.00	0.44
1:A:385:THR:HG23	1:A:386:LYS:HG3	2.00	0.44
3:H:83:MET:HE2	3:H:86:LEU:HD21	2.00	0.44
3:C:67:ARG:NH2	3:C:90:ASP:OD2	2.49	0.44
2:F:23:CYS:HB2	2:F:40:TRP:CH2	2.53	0.43
2:F:40:TRP:CE2	2:F:78:LEU:HG	2.53	0.43
2:B:173:GLN:HG3	2:B:180:TYR:CZ	2.54	0.43
1:E:396:TYR:HB2	1:E:514:SER:HB2	2.00	0.43
2:F:127:PRO:HD3	2:F:139:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:386:LYS:O	1:E:390:LEU:HG	2.19	0.42
2:L:173:GLN:HG3	2:L:180:TYR:CZ	2.54	0.42
2:B:144:ASN:ND2	3:C:199:THR:HG21	2.34	0.42
1:A:338:PHE:CD2	1:A:368:LEU:HD21	2.54	0.42
2:B:66:ARG:HD2	2:B:82:ARG:O	2.20	0.42
1:D:385:THR:HG23	1:D:386:LYS:HG3	2.01	0.42
3:H:18:LEU:HD23	3:H:86:LEU:HD11	2.02	0.42
1:A:350:VAL:HA	1:A:400:PHE:HB2	2.01	0.42
3:C:29:PHE:CE1	3:C:34:MET:HE3	2.55	0.42
1:D:440:ASN:OD1	1:D:440:ASN:N	2.53	0.42
2:F:2:ILE:HG23	2:F:27:GLN:HG2	2.01	0.42
3:G:51:ILE:HG13	3:G:70:ILE:HD13	2.02	0.42
2:B:40:TRP:CD2	2:B:78:LEU:HG	2.54	0.42
3:G:12:VAL:HG13	3:G:127:VAL:HG22	2.02	0.42
2:L:71:GLY:HA3	2:L:76:PHE:HA	2.02	0.41
1:A:444:LYS:HG3	3:C:114:TYR:CG	2.55	0.41
1:D:384:PRO:HA	1:D:387:LEU:HG	2.01	0.41
2:F:30:LEU:HD23	2:F:31:HIS:O	2.21	0.41
3:H:4:LEU:HD22	3:H:22:CYS:SG	2.60	0.41
3:C:18:LEU:HD23	3:C:86:LEU:HD11	2.02	0.41
1:D:350:VAL:HG22	1:D:422:ASN:HB3	2.02	0.41
2:L:40:TRP:CE2	2:L:78:LEU:HG	2.56	0.41
1:D:371:SER:C	1:D:373:SER:H	2.28	0.41
2:L:40:TRP:CD2	2:L:78:LEU:HG	2.56	0.40
3:H:148:SER:HG	3:H:149:GLY:H	1.67	0.40
3:G:184:ALA:HA	3:G:194:LEU:HB3	2.02	0.40
2:L:59:ARG:HD3	2:L:67:PHE:O	2.21	0.40
1:D:396:TYR:O	1:D:513:LEU:HA	2.22	0.40

All (1) 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)
2:L:117:VAL:O	2:B:156:LYS:NZ[4_444]	2.18	0.02

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	197/205 (96%)	189 (96%)	8 (4%)	0	100	100
1	D	195/205 (95%)	187 (96%)	8 (4%)	0	100	100
1	E	195/205 (95%)	185 (95%)	10 (5%)	0	100	100
2	B	217/221 (98%)	211 (97%)	6 (3%)	0	100	100
2	F	215/221 (97%)	211 (98%)	4 (2%)	0	100	100
2	L	219/221 (99%)	211 (96%)	8 (4%)	0	100	100
3	C	219/234 (94%)	211 (96%)	7 (3%)	1 (0%)	24	53
3	G	185/234 (79%)	170 (92%)	14 (8%)	1 (0%)	24	53
3	H	226/234 (97%)	214 (95%)	11 (5%)	1 (0%)	30	58
All	All	1868/1980 (94%)	1789 (96%)	76 (4%)	3 (0%)	43	71

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	160	ASP
3	G	165	PRO
3	H	160	ASP

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	171/177 (97%)	169 (99%)	2 (1%)	63	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	170/177 (96%)	166 (98%)	4 (2%)	43	73
1	E	170/177 (96%)	170 (100%)	0	100	100
2	B	193/195 (99%)	193 (100%)	0	100	100
2	F	192/195 (98%)	191 (100%)	1 (0%)	81	93
2	L	195/195 (100%)	195 (100%)	0	100	100
3	C	184/194 (95%)	183 (100%)	1 (0%)	81	93
3	G	158/194 (81%)	154 (98%)	4 (2%)	42	73
3	H	188/194 (97%)	187 (100%)	1 (0%)	81	93
All	All	1621/1698 (96%)	1608 (99%)	13 (1%)	73	89

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	H	109	VAL
1	A	382	VAL
1	A	511	VAL
3	C	102	ILE
1	D	333	THR
1	D	382	VAL
1	D	472	ILE
1	D	511	VAL
2	F	39	ASP
3	G	51	ILE
3	G	102	ILE
3	G	133	LYS
3	G	221	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	330	HIS
1	E	519	HIS
2	L	144	ASN
2	L	217	ASN
3	H	74	ASN
3	H	77	ASN
1	A	330	HIS
1	A	394	ASN

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Mol	Chain	Res	Type
2	B	196	HIS
3	C	74	ASN
3	C	121	GLN
2	F	36	ASN
2	F	144	ASN
2	F	196	HIS
2	F	206	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 3 are monoatomic - leaving 11 for Mogul analysis.

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	$\# Z > 2$
8	GOL	B	301	-	5,5,5	0.89	0	5,5,5	1.04	0
8	GOL	F	301	-	5,5,5	0.90	0	5,5,5	1.05	0
6	NO3	C	301	-	1,3,3	0.56	0	0,3,3	-	-
4	NAG	D	601	1	14,14,15	0.37	0	17,19,21	0.57	0
4	NAG	E	601	1	14,14,15	0.31	0	17,19,21	0.53	0
4	NAG	A	601	1	14,14,15	0.56	0	17,19,21	0.89	1 (5%)
6	NO3	L	301	-	1,3,3	0.50	0	0,3,3	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	L	302	-	4,4,4	0.25	0	6,6,6	0.13	0
5	SO4	H	402	-	4,4,4	0.22	0	6,6,6	0.09	0
5	SO4	E	602	-	4,4,4	0.23	0	6,6,6	0.11	0
6	NO3	H	401	-	1,3,3	0.49	0	0,3,3	-	-

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
8	GOL	B	301	-	-	2/4/4/4	-
8	GOL	F	301	-	-	4/4/4/4	-
4	NAG	D	601	1	-	0/6/23/26	0/1/1/1
4	NAG	E	601	1	-	2/6/23/26	0/1/1/1
4	NAG	A	601	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	NAG	C1-O5-C5	3.25	116.54	112.19

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	F	301	GOL	O1-C1-C2-C3
4	A	601	NAG	O5-C5-C6-O6
4	E	601	NAG	O5-C5-C6-O6
4	A	601	NAG	C4-C5-C6-O6
4	E	601	NAG	C4-C5-C6-O6
8	B	301	GOL	C1-C2-C3-O3
8	F	301	GOL	C1-C2-C3-O3
8	F	301	GOL	O1-C1-C2-O2
8	F	301	GOL	O2-C2-C3-O3
8	B	301	GOL	O2-C2-C3-O3

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	199/205 (97%)	-0.35	1 (0%) 87 83	92, 114, 187, 223	0
1	D	197/205 (96%)	-0.34	0 100 100	86, 119, 203, 230	0
1	E	197/205 (96%)	-0.35	2 (1%) 79 72	91, 110, 188, 223	0
2	B	219/221 (99%)	-0.40	0 100 100	92, 118, 160, 209	0
2	F	217/221 (98%)	-0.29	2 (0%) 81 74	103, 167, 224, 243	0
2	L	221/221 (100%)	-0.49	0 100 100	88, 105, 137, 195	0
3	C	223/234 (95%)	-0.33	0 100 100	88, 122, 156, 171	0
3	G	191/234 (81%)	-0.37	0 100 100	83, 111, 206, 329	0
3	H	228/234 (97%)	-0.46	0 100 100	89, 115, 151, 192	0
All	All	1892/1980 (95%)	-0.38	5 (0%) 90 87	83, 117, 194, 329	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	329	HIS	2.8
1	A	341	VAL	2.6
2	F	140	VAL	2.6
2	F	142	LEU	2.5
1	E	356	LYS	2.3

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

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	NAG	A	601	14/15	0.59	0.13	195,202,217,218	0
4	NAG	E	601	14/15	0.70	0.10	141,171,186,190	0
5	SO4	H	402	5/5	0.72	0.07	187,188,202,288	0
4	NAG	D	601	14/15	0.73	0.10	126,165,180,190	0
5	SO4	E	602	5/5	0.77	0.07	160,177,201,328	0
6	NO3	C	301	4/4	0.78	0.10	131,134,135,138	0
5	SO4	L	302	5/5	0.88	0.10	158,173,192,194	0
6	NO3	H	401	4/4	0.89	0.06	123,128,131,139	0
6	NO3	L	301	4/4	0.89	0.08	118,121,121,123	0
7	CL	G	301	1/1	0.89	0.08	117,117,117,117	0
8	GOL	F	301	6/6	0.89	0.12	129,137,138,141	0
7	CL	L	303	1/1	0.90	0.07	116,116,116,116	0
7	CL	H	403	1/1	0.91	0.07	119,119,119,119	0
8	GOL	B	301	6/6	0.94	0.10	116,117,121,122	0

6.5 Other polymers

There are no such residues in this entry.