Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2020 – 10:28 pm BST

PDB ID	:	6OE4
Title	:	Prefusion RSV F monomer bound by neutralizing antibody CR9501
Authors	:	McLellan, J.S.; Gilman, M.S.A.
Deposited on	:	2019-03-27
Resolution	:	3.30 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 following versions of software and data (see references ⓘ) were used in the production of this report:

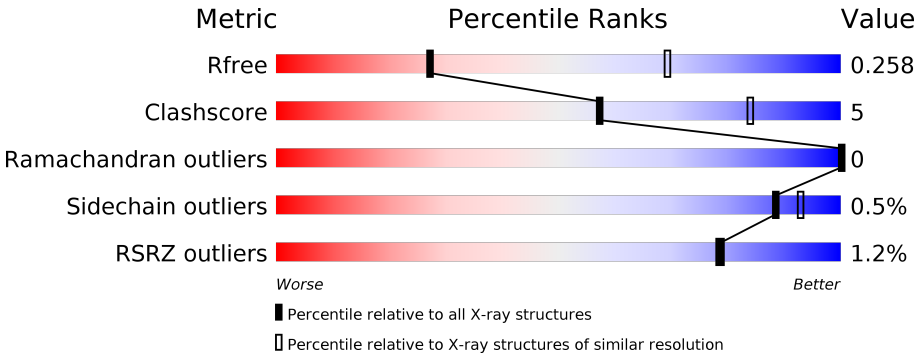
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 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	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 on 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	521	2% 72% 9% 18%
1	D	521	2% 69% 13% 17%
2	C	214	88% 11%
2	F	214	93% 7%
3	B	230	87% 11%
3	E	230	83% 14%

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	EDO	C	302	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13310 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 Fusion glycoprotein F0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	0	0
			3321	2098	545	655	23			
1	D	430	Total	C	N	O	S	0	0	0
			3339	2109	549	658	23			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	PRO	conflict	UNP P03420
A	155	CYS	SER	engineered mutation	UNP P03420
A	190	PHE	SER	engineered mutation	UNP P03420
A	207	LEU	VAL	engineered mutation	UNP P03420
A	290	CYS	SER	engineered mutation	UNP P03420
A	379	VAL	ILE	conflict	UNP P03420
A	447	VAL	MET	conflict	UNP P03420
A	514	GLY	-	expression tag	UNP P03420
A	515	SER	-	expression tag	UNP P03420
A	516	LEU	-	expression tag	UNP P03420
A	517	GLU	-	expression tag	UNP P03420
A	518	VAL	-	expression tag	UNP P03420
A	519	LEU	-	expression tag	UNP P03420
A	520	PHE	-	expression tag	UNP P03420
A	521	GLN	-	expression tag	UNP P03420
D	102	ALA	PRO	conflict	UNP P03420
D	155	CYS	SER	engineered mutation	UNP P03420
D	190	PHE	SER	engineered mutation	UNP P03420
D	207	LEU	VAL	engineered mutation	UNP P03420
D	290	CYS	SER	engineered mutation	UNP P03420
D	379	VAL	ILE	conflict	UNP P03420
D	447	VAL	MET	conflict	UNP P03420
D	514	GLY	-	expression tag	UNP P03420
D	515	SER	-	expression tag	UNP P03420
D	516	LEU	-	expression tag	UNP P03420

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Chain	Residue	Modelled	Actual	Comment	Reference
D	517	GLU	-	expression tag	UNP P03420
D	518	VAL	-	expression tag	UNP P03420
D	519	LEU	-	expression tag	UNP P03420
D	520	PHE	-	expression tag	UNP P03420
D	521	GLN	-	expression tag	UNP P03420

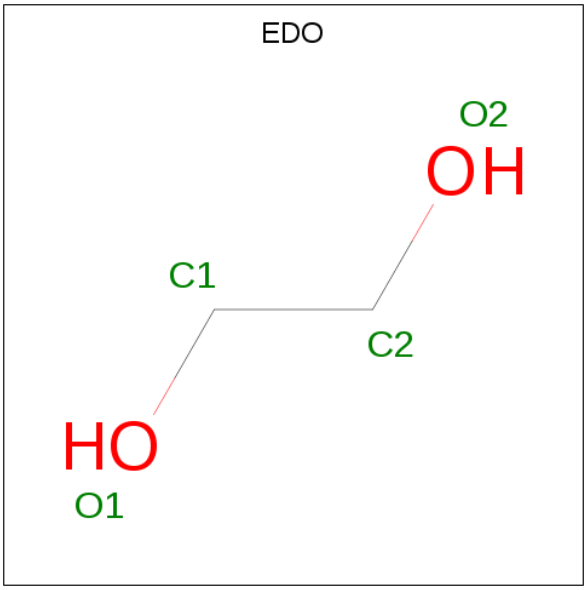
- Molecule 2 is a protein called CR9501 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	212	Total	C	N	O	S	0	0	0
			1641	1032	270	334	5			
2	F	212	Total	C	N	O	S	0	0	0
			1641	1032	270	334	5			

- Molecule 3 is a protein called CR9501 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	225	Total	C	N	O	S	0	0	0
			1674	1058	279	330	7			
3	E	225	Total	C	N	O	S	0	0	0
			1674	1058	279	330	7			

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



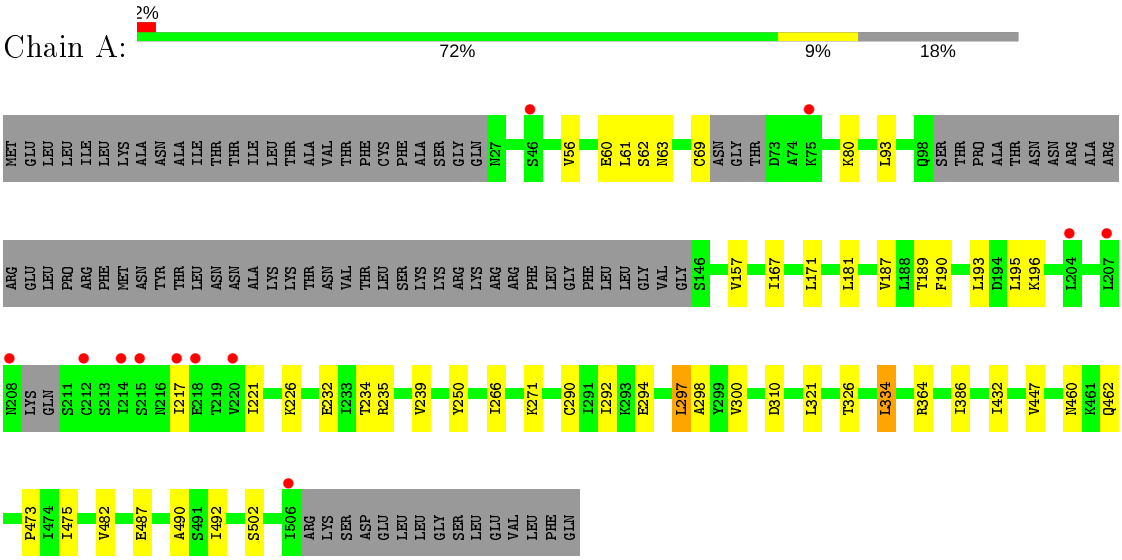
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

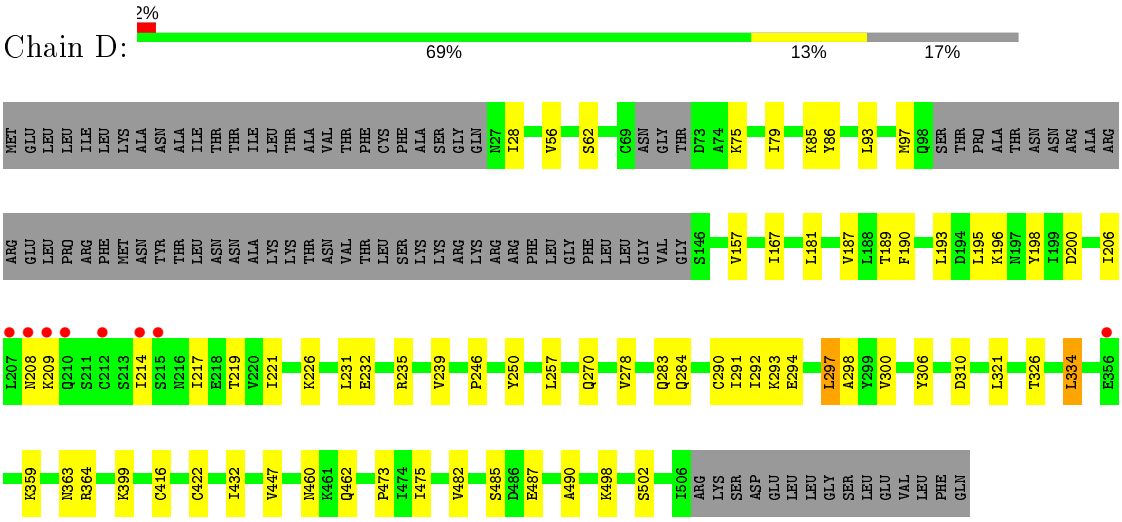
- Molecule 1: Fusion glycoprotein F0

Chain A:



- Molecule 1: Fusion glycoprotein F0

Chain D:

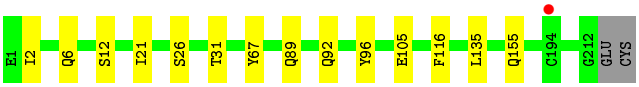


- Molecule 2: CR9501 Fab Light Chain

Chain C:

• Molecule 2: CR9501 Fab Light Chain

Chain F:

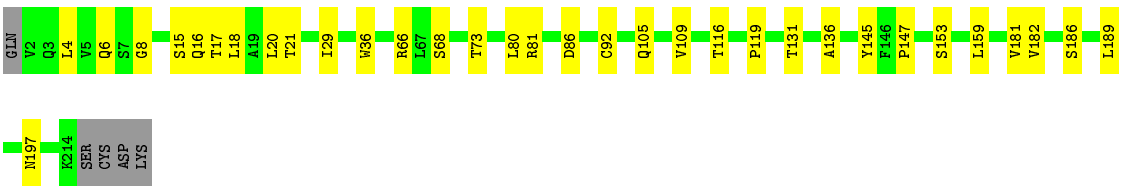


• Molecule 3: CR9501 Fab Heavy Chain

Chain B:

• Molecule 3: CR9501 Fab Heavy Chain

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	105.63Å 153.39Å 155.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.81 – 3.30 52.81 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (52.81-3.30) 99.4 (52.81-3.30)	Depositor EDS
R_{merge}	0.39	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.212 , 0.259 0.212 , 0.258	Depositor DCC
R_{free} test set	1819 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å^2)	61.6	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 32.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13310	wwPDB-VP
Average B, all atoms (Å^2)	60.0	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 40.72 % 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 2.6237e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: 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	A	0.32	0/3367	0.58	1/4561 (0.0%)
1	D	0.33	1/3386 (0.0%)	0.60	2/4587 (0.0%)
2	C	0.28	0/1678	0.48	0/2285
2	F	0.28	0/1678	0.48	0/2285
3	B	0.27	0/1717	0.48	0/2349
3	E	0.28	0/1717	0.49	0/2349
All	All	0.30	1/13543 (0.0%)	0.54	3/18416 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	416	CYS	CB-SG	-5.84	1.72	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	422	CYS	CA-CB-SG	8.21	128.78	114.00
1	A	334	LEU	CA-CB-CG	6.17	129.49	115.30
1	D	334	LEU	CA-CB-CG	6.07	129.26	115.30

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	3321	0	3355	32	0
1	D	3339	0	3377	44	0
2	C	1641	0	1590	16	1
2	F	1641	0	1590	10	0
3	B	1674	0	1635	15	0
3	E	1674	0	1635	17	1
4	C	8	0	12	1	0
4	D	4	0	6	0	0
4	F	8	0	12	1	0
All	All	13310	0	13212	130	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 5.

All (130) 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:482:VAL:HG13	1:A:502:SER:HB2	1.59	0.85
2:C:108:ARG:HH12	2:C:111:ALA:HB2	1.41	0.84
1:D:482:VAL:HG13	1:D:502:SER:HB2	1.60	0.83
1:D:310:ASP:OD1	1:D:364:ARG:NH1	2.12	0.81
1:D:321:LEU:HD11	1:D:473:PRO:HB3	1.65	0.79
1:A:294:GLU:OE1	2:C:92:GLN:NE2	2.20	0.74
1:D:294:GLU:OE1	2:F:92:GLN:NE2	2.21	0.74
1:D:193:LEU:HD11	1:D:226:LYS:HG2	1.71	0.71
1:D:432:ILE:HD11	1:D:447:VAL:HG22	1.72	0.71
1:A:321:LEU:HD11	1:A:473:PRO:HB3	1.72	0.71
3:E:8:GLY:HA3	3:E:20:LEU:HD23	1.71	0.70
2:C:108:ARG:HD2	2:C:171:SER:HB2	1.74	0.69
1:D:56:VAL:HG23	1:D:187:VAL:HG11	1.76	0.68
1:A:56:VAL:HG23	1:A:187:VAL:HG11	1.77	0.66
1:A:193:LEU:HD11	1:A:226:LYS:HG2	1.77	0.66
3:B:8:GLY:HA3	3:B:20:LEU:HD23	1.78	0.66
1:D:93:LEU:HB3	1:D:292:ILE:HD12	1.78	0.65
1:A:432:ILE:HD11	1:A:447:VAL:HG22	1.77	0.64
1:A:232:GLU:HG2	1:A:250:TYR:CD2	2.34	0.62
2:F:155:GLN:HE22	4:F:301:EDO:H12	1.63	0.62
1:D:232:GLU:HG2	1:D:250:TYR:CD2	2.35	0.62
3:B:16:GLN:HG3	3:B:17:THR:H	1.64	0.62
1:D:198:TYR:OH	1:D:219:THR:O	2.19	0.61
1:A:93:LEU:HB3	1:A:292:ILE:HD12	1.82	0.60
2:C:211:ARG:NH1	4:C:302:EDO:O2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:6:GLN:H	3:E:105:GLN:HE22	1.51	0.57
1:A:334:LEU:HB2	1:A:475:ILE:HD13	1.88	0.56
1:A:157:VAL:HG11	1:A:181:LEU:HB3	1.88	0.56
1:D:399:LYS:HE3	1:D:485:SER:OG	2.05	0.56
1:D:79:ILE:HD11	1:D:214:ILE:HG21	1.88	0.56
3:E:159:LEU:HD21	3:E:182:VAL:HG11	1.89	0.55
2:C:31:THR:HG23	2:C:67:TYR:HD2	1.71	0.55
1:D:460:ASN:OD1	1:D:462:GLN:HG3	2.07	0.55
3:E:181:VAL:HG11	2:F:135:LEU:HD22	1.89	0.55
1:A:235:ARG:O	1:A:239:VAL:HG23	2.08	0.54
3:B:131:THR:HG22	3:B:136:ALA:HB2	1.89	0.54
1:D:217:ILE:O	1:D:221:ILE:HG13	2.09	0.53
3:E:16:GLN:HG2	3:E:17:THR:H	1.72	0.53
3:E:68:SER:HB3	3:E:81:ARG:HB2	1.90	0.53
2:C:31:THR:HG23	2:C:67:TYR:CD2	2.45	0.52
1:A:460:ASN:OD1	1:A:462:GLN:NE2	2.43	0.51
1:A:93:LEU:HD13	1:A:292:ILE:HD11	1.93	0.51
1:A:217:ILE:O	1:A:221:ILE:HG13	2.11	0.51
2:C:108:ARG:HH12	2:C:111:ALA:CB	2.18	0.50
1:D:167:ILE:HG23	1:D:189:THR:HG21	1.93	0.50
1:D:97:MET:SD	1:D:291:ILE:HA	2.52	0.50
3:B:6:GLN:H	3:B:105:GLN:HE22	1.60	0.50
1:A:69:CYS:HB2	1:A:80:LYS:NZ	2.27	0.50
3:E:131:THR:HG22	3:E:136:ALA:HB2	1.93	0.50
1:D:290:CYS:SG	1:D:300:VAL:HG23	2.52	0.50
1:D:157:VAL:HG11	1:D:181:LEU:HB3	1.93	0.49
1:D:75:LYS:HE2	1:D:217:ILE:HG12	1.93	0.49
3:E:36:TRP:CE2	3:E:80:LEU:HB2	2.47	0.49
1:D:334:LEU:HB2	1:D:475:ILE:HD13	1.94	0.49
3:B:153:SER:HB2	3:B:197:ASN:HB2	1.94	0.49
2:F:116:PHE:HD2	2:F:135:LEU:HD23	1.77	0.49
2:C:135:LEU:HD22	3:B:181:VAL:HG11	1.95	0.49
2:C:193:ALA:HB2	2:C:208:SER:HB3	1.96	0.48
1:A:62:SER:OG	1:A:63:ASN:N	2.46	0.48
1:D:235:ARG:O	1:D:239:VAL:HG23	2.14	0.48
2:F:31:THR:HG23	2:F:67:TYR:HD1	1.78	0.48
3:E:119:PRO:HB3	3:E:145:TYR:HB3	1.96	0.48
3:B:116:THR:HG22	3:B:147:PRO:HD3	1.95	0.47
1:D:257:LEU:HD23	1:D:278:VAL:HG13	1.94	0.47
1:D:487:GLU:HB3	1:D:490:ALA:HB2	1.96	0.47
3:E:18:LEU:HD12	3:E:109:VAL:HG11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:CYS:SG	1:A:300:VAL:HG23	2.54	0.47
1:D:482:VAL:HG13	1:D:502:SER:CB	2.39	0.47
3:E:29:ILE:HG21	3:E:73:THR:HA	1.97	0.47
1:D:206:ILE:HG21	1:D:214:ILE:HD11	1.96	0.46
3:B:60:THR:HG22	3:B:62:SER:H	1.79	0.46
3:B:68:SER:HB3	3:B:81:ARG:HB2	1.97	0.46
1:D:487:GLU:OE2	1:D:498:LYS:NZ	2.36	0.46
1:D:293:LYS:HG2	1:D:294:GLU:HG3	1.97	0.46
3:E:66:ARG:NH2	3:E:86:ASP:OD2	2.50	0.45
2:C:19:VAL:HG21	2:C:78:LEU:HD22	1.98	0.45
1:A:61:LEU:O	1:A:196:LYS:HB2	2.16	0.45
1:D:291:ILE:HD11	1:D:293:LYS:HE3	1.97	0.45
1:D:270:GLN:NE2	1:D:306:TYR:O	2.44	0.45
1:A:195:LEU:HD21	1:A:226:LYS:HB3	1.99	0.45
1:A:310:ASP:OD1	1:A:364:ARG:NH1	2.32	0.45
1:A:167:ILE:HG23	1:A:189:THR:HG21	1.98	0.45
1:D:93:LEU:HD13	1:D:292:ILE:HD11	1.98	0.45
1:A:487:GLU:HB3	1:A:490:ALA:HB2	1.99	0.45
1:D:246:PRO:HB3	1:D:283:GLN:HA	1.98	0.45
2:F:31:THR:HG23	2:F:67:TYR:CD1	2.52	0.45
1:D:284:GLN:CG	1:D:359:LYS:HE3	2.48	0.44
1:A:62:SER:HB2	1:A:196:LYS:HA	1.98	0.44
1:A:60:GLU:OE1	1:A:196:LYS:HD3	2.17	0.44
3:B:21:THR:HG22	3:B:79:SER:HB3	2.00	0.44
1:A:171:LEU:HD11	1:A:189:THR:HG22	2.00	0.44
1:A:69:CYS:HB2	1:A:80:LYS:HZ2	1.82	0.43
1:D:79:ILE:CD1	1:D:214:ILE:HG21	2.48	0.43
3:E:116:THR:HG22	3:E:147:PRO:HD3	2.00	0.43
3:E:153:SER:HB2	3:E:197:ASN:HB2	1.99	0.43
3:E:18:LEU:CD1	3:E:109:VAL:HG11	2.48	0.43
1:D:62:SER:O	1:D:86:TYR:OH	2.34	0.43
2:F:2:ILE:HG23	2:F:26:SER:HB3	1.99	0.43
1:A:297:LEU:HD12	1:A:298:ALA:N	2.34	0.43
1:A:482:VAL:HG13	1:A:502:SER:CB	2.39	0.43
1:D:292:ILE:HG12	1:D:297:LEU:HA	2.00	0.42
1:A:482:VAL:O	1:A:482:VAL:HG12	2.17	0.42
1:D:482:VAL:O	1:D:482:VAL:HG12	2.19	0.42
2:F:6:GLN:HE21	2:F:21:ILE:HG21	1.84	0.42
3:B:4:LEU:HD13	3:B:92:CYS:SG	2.60	0.42
2:C:150:VAL:HG22	2:C:192:TYR:CD2	2.55	0.42
3:E:186:SER:O	3:E:189:LEU:HG	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:119:PRO:HD2	3:B:205:THR:HG21	2.02	0.42
2:C:23:CYS:HB2	2:C:35:TRP:CH2	2.54	0.42
2:C:12:SER:HA	2:C:105:GLU:O	2.20	0.41
2:C:89:GLN:HB2	2:C:98:PHE:CD2	2.55	0.41
1:D:206:ILE:HG21	1:D:214:ILE:CD1	2.50	0.41
1:D:208:ASN:OD1	1:D:209:LYS:HG3	2.20	0.41
1:A:386:ILE:HG12	1:A:492:ILE:HD11	2.02	0.41
1:D:28:ILE:HD11	1:D:363:ASN:HB2	2.02	0.41
1:D:196:LYS:HE3	1:D:200:ASP:OD2	2.21	0.41
3:B:159:LEU:HD21	3:B:182:VAL:HG11	2.02	0.41
2:F:89:GLN:HE21	2:F:96:TYR:HB3	1.84	0.41
1:A:93:LEU:HG	1:A:234:THR:HG23	2.03	0.41
1:A:266:ILE:HG13	1:A:271:LYS:HG3	2.03	0.41
2:F:12:SER:HA	2:F:105:GLU:O	2.20	0.41
2:C:192:TYR:HB2	2:C:209:PHE:CE1	2.56	0.41
1:D:214:ILE:HD13	1:D:214:ILE:HA	1.85	0.41
3:E:4:LEU:HD13	3:E:92:CYS:SG	2.61	0.41
1:D:195:LEU:HD21	1:D:226:LYS:HB3	2.03	0.41
1:D:85:LYS:HD3	1:D:231:LEU:HD11	2.04	0.40
3:B:119:PRO:HB3	3:B:145:TYR:HB3	2.02	0.40
1:D:297:LEU:HD12	1:D:298:ALA:N	2.36	0.40
3:B:6:GLN:HB3	3:B:6:GLN:HE21	1.75	0.40
2:C:115:VAL:O	2:C:207:LYS:HE3	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:C:109:THR:OG1	3:E:15:SER:OG[1_455]	2.18	0.02

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	420/521 (81%)	410 (98%)	10 (2%)	0	100	100
1	D	424/521 (81%)	412 (97%)	12 (3%)	0	100	100
2	C	210/214 (98%)	202 (96%)	8 (4%)	0	100	100
2	F	210/214 (98%)	203 (97%)	7 (3%)	0	100	100
3	B	223/230 (97%)	217 (97%)	6 (3%)	0	100	100
3	E	223/230 (97%)	216 (97%)	7 (3%)	0	100	100
All	All	1710/1930 (89%)	1660 (97%)	50 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	393/473 (83%)	390 (99%)	3 (1%)	81	89
1	D	395/473 (84%)	392 (99%)	3 (1%)	81	89
2	C	187/189 (99%)	187 (100%)	0	100	100
2	F	187/189 (99%)	187 (100%)	0	100	100
3	B	191/196 (97%)	191 (100%)	0	100	100
3	E	191/196 (97%)	190 (100%)	1 (0%)	88	93
All	All	1544/1716 (90%)	1537 (100%)	7 (0%)	88	93

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	190	PHE
1	A	297	LEU
1	A	326	THR
1	D	190	PHE
1	D	297	LEU
1	D	326	THR
3	E	21	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	F	155	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

5 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	D	601	-	3,3,3	0.45	0	2,2,2	0.27	0
4	EDO	C	302	-	3,3,3	0.46	0	2,2,2	0.33	0
4	EDO	F	302	-	3,3,3	0.48	0	2,2,2	0.31	0
4	EDO	F	301	-	3,3,3	0.46	0	2,2,2	0.33	0
4	EDO	C	301	-	3,3,3	0.46	0	2,2,2	0.32	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	D	601	-	-	0/1/1/1	-
4	EDO	C	302	-	-	0/1/1/1	-
4	EDO	F	302	-	-	0/1/1/1	-
4	EDO	F	301	-	-	0/1/1/1	-
4	EDO	C	301	-	-	0/1/1/1	-

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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	302	EDO	1	0
4	F	301	EDO	1	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, 95^{th} 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	428/521 (82%)	0.34	12 (2%) 53 51	34, 67, 135, 191	0
1	D	430/521 (82%)	0.31	8 (1%) 66 65	35, 63, 118, 188	0
2	C	212/214 (99%)	-0.04	0 100 100	25, 47, 73, 86	0
2	F	212/214 (99%)	-0.07	1 (0%) 91 91	25, 46, 73, 100	0
3	B	225/230 (97%)	0.06	0 100 100	29, 56, 85, 119	0
3	E	225/230 (97%)	-0.09	0 100 100	25, 46, 83, 112	0
All	All	1732/1930 (89%)	0.15	21 (1%) 79 78	25, 55, 113, 191	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	210	GLN	5.3
1	A	208	ASN	5.0
1	D	208	ASN	4.5
1	A	207	LEU	3.5
1	A	215	SER	3.2
1	D	207	LEU	3.1
1	D	214	ILE	3.0
1	D	356	GLU	2.9
1	D	209	LYS	2.9
1	A	214	ILE	2.8
1	D	212	CYS	2.8
1	A	217	ILE	2.6
1	A	204	LEU	2.6
1	A	506	ILE	2.5
1	A	220	VAL	2.5
1	A	212	CYS	2.4
1	D	215	SER	2.4
1	A	218	GLU	2.2
2	F	194	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	75	LYS	2.0
1	A	46	SER	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 carbohydrates 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, 95^{th} 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	C	302	4/4	0.74	0.43	48,49,52,52	0
4	EDO	F	302	4/4	0.81	0.43	39,40,41,41	0
4	EDO	D	601	4/4	0.82	0.47	50,50,51,53	0
4	EDO	F	301	4/4	0.88	0.62	57,57,57,57	0
4	EDO	C	301	4/4	0.93	0.46	38,39,39,40	0

6.5 Other polymers (i)

There are no such residues in this entry.