



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 10:38 AM BST

PDB ID : 6DC5
Title : RSV prefusion F in complex with AM22 Fab
Authors : Jones, H.G.; McLellan, J.S.
Deposited on : 2018-05-04
Resolution : 3.50 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 : 2.13.1
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) : 2.13.1

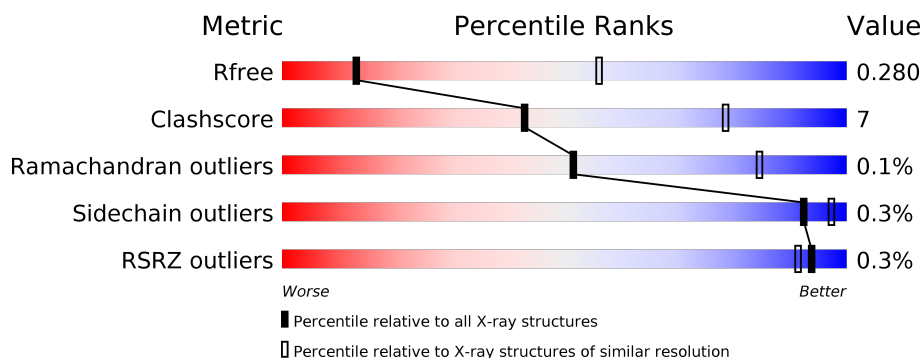
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 $\leq 5\%$. 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	568	
1	D	568	
1	G	568	
2	B	228	
2	E	228	
2	H	228	

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Mol	Chain	Length	Quality of chain
3	C	215	 85% 14% .
3	F	215	 84% 15% .
3	I	215	 79% 20%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 20286 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 RSV fusion glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	445	Total	C	N	O	S	0	0	0
			3449	2181	569	676	23			
1	D	449	Total	C	N	O	S	0	0	0
			3483	2201	574	685	23			
1	G	444	Total	C	N	O	S	0	0	0
			3440	2176	567	674	23			

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	PRO	variant	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	variant	UNP P03420
A	447	VAL	MET	variant	UNP P03420
A	514	SER	-	linker	UNP P03420
A	515	ALA	-	linker	UNP P03420
A	516	ILE	-	linker	UNP P03420
A	517	GLY	-	linker	UNP P03420
D	102	ALA	PRO	variant	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	variant	UNP P03420
D	447	VAL	MET	variant	UNP P03420
D	514	SER	-	linker	UNP P03420
D	515	ALA	-	linker	UNP P03420
D	516	ILE	-	linker	UNP P03420
D	517	GLY	-	linker	UNP P03420
G	102	ALA	PRO	variant	UNP P03420

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Chain	Residue	Modelled	Actual	Comment	Reference
G	155	CYS	SER	engineered mutation	UNP P03420
G	190	PHE	SER	engineered mutation	UNP P03420
G	207	LEU	VAL	engineered mutation	UNP P03420
G	290	CYS	SER	engineered mutation	UNP P03420
G	379	VAL	ILE	variant	UNP P03420
G	447	VAL	MET	variant	UNP P03420
G	514	SER	-	linker	UNP P03420
G	515	ALA	-	linker	UNP P03420
G	516	ILE	-	linker	UNP P03420
G	517	GLY	-	linker	UNP P03420

- Molecule 2 is a protein called Fab AM22 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	221	Total	C	N	O	S	0	0	0
			1646	1046	271	323	6			
2	E	221	Total	C	N	O	S	0	0	0
			1646	1046	271	323	6			
2	H	223	Total	C	N	O	S	0	0	0
			1658	1052	273	326	7			

- Molecule 3 is a protein called Fab AM22 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	213	Total	C	N	O	S	0	0	0
			1622	1019	277	322	4			
3	F	212	Total	C	N	O	S	0	0	0
			1618	1017	276	321	4			
3	I	215	Total	C	N	O	S	0	0	0
			1637	1027	279	326	5			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

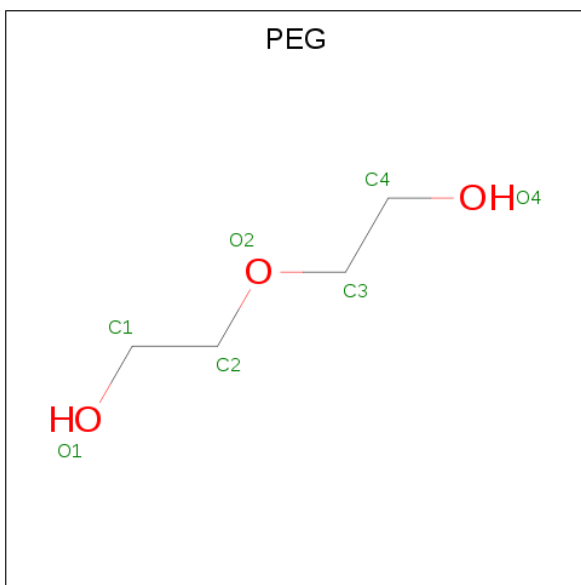


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	Cd	0	0
			1	1		
5	A	1	Total	Cd	0	0
			1	1		
5	D	1	Total	Cd	0	0
			1	1		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).

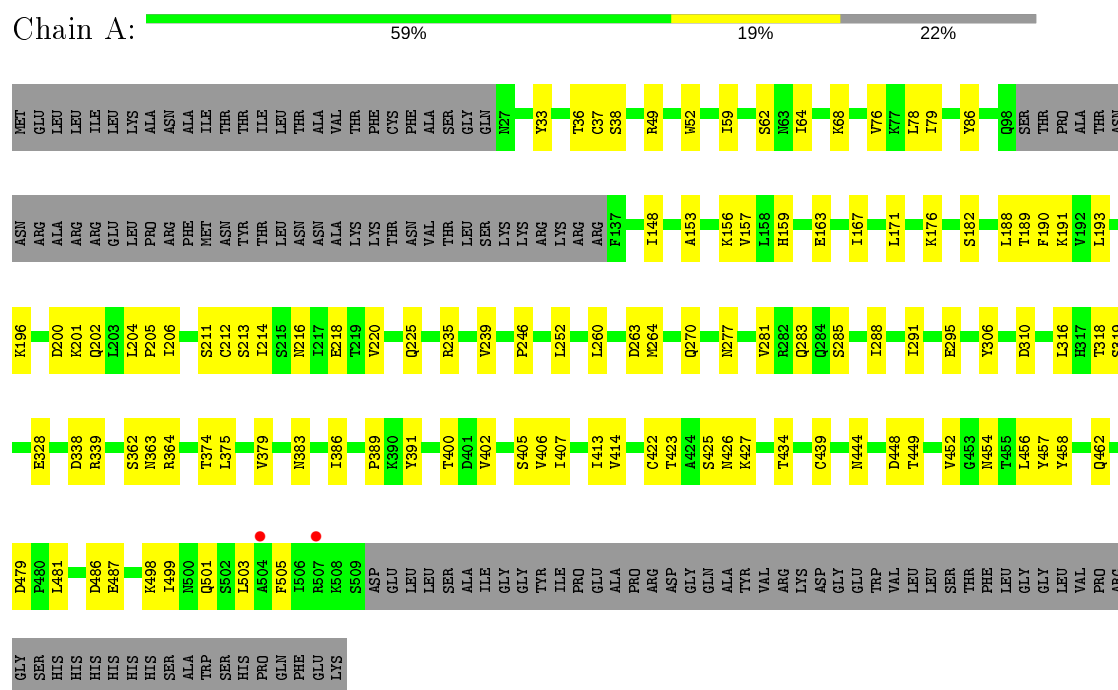


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			7	4	3		
6	C	1	Total	C	O	0	0
			7	4	3		
6	F	1	Total	C	O	0	0
			7	4	3		
6	F	1	Total	C	O	0	0
			7	4	3		
6	I	1	Total	C	O	0	0
			7	4	3		
6	I	1	Total	C	O	0	0
			7	4	3		

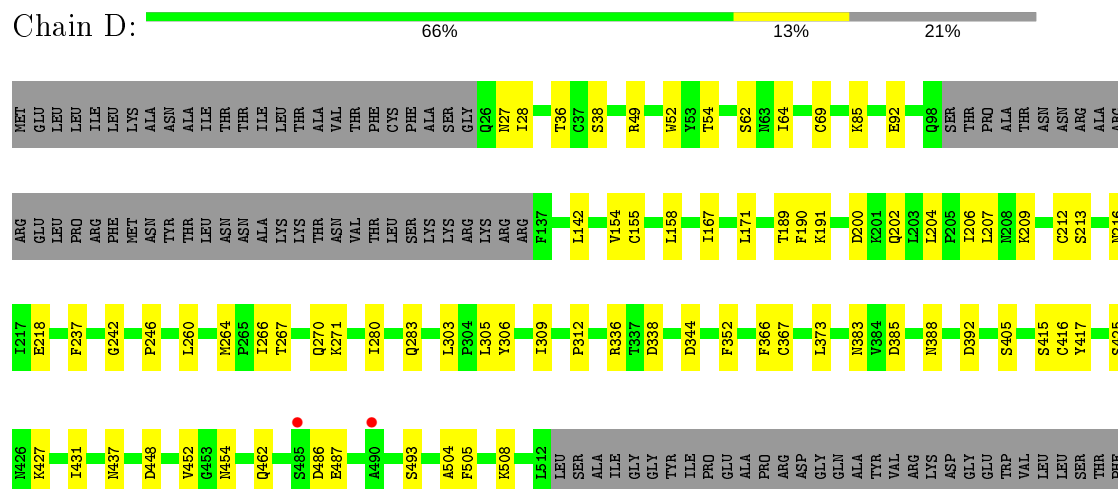
3 Residue-property plots [i](#)

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: RSV fusion glycoprotein

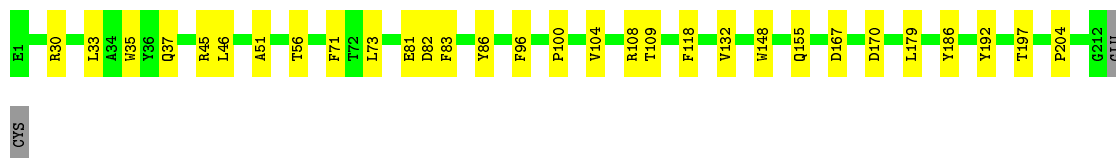


• Molecule 1: RSV fusion glycoprotein




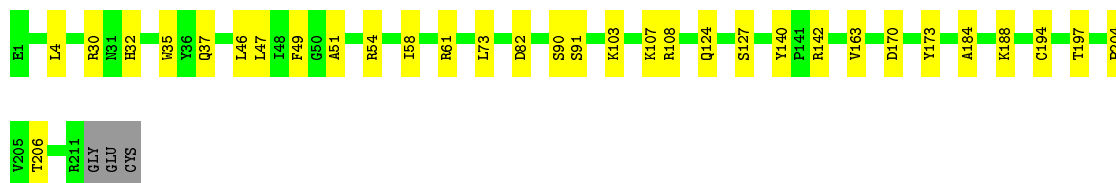
- Molecule 3: Fab AM22 light chain

Chain C:  85% 14%




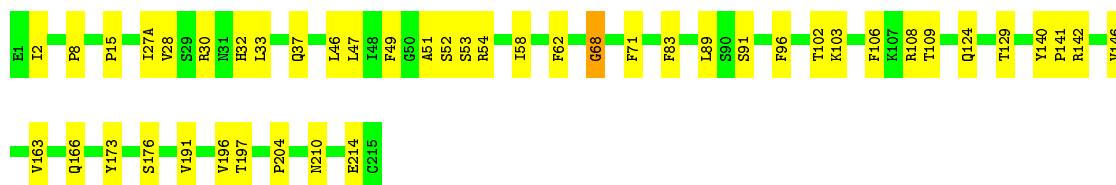
- Molecule 3: Fab AM22 light chain

Chain F:  84% 15%



- Molecule 3: Fab AM22 light chain

Chain I:  79% 20%



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	132.45Å 152.18Å 202.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.23 – 3.50 47.23 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.23-3.50) 99.8 (47.23-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, R_{free}	0.217 , 0.280 0.217 , 0.280	Depositor DCC
R_{free} test set	2606 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	58.6	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	20286	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% 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: PEG, NAG, CD

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	0.26	0/3499	0.45	0/4739
1	D	0.25	0/3533	0.45	0/4785
1	G	0.25	0/3490	0.45	0/4727
2	B	0.27	0/1682	0.50	0/2292
2	E	0.26	0/1682	0.50	0/2292
2	H	0.27	0/1694	0.50	0/2308
3	C	0.34	1/1658 (0.1%)	0.49	0/2252
3	F	0.29	0/1654	0.51	0/2247
3	I	0.30	0/1673	0.49	0/2272
All	All	0.27	1/20565 (0.0%)	0.47	0/27914

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	100	PRO	N-CD	-6.73	1.38	1.47

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	3449	0	3493	82	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3483	0	3522	60	0
1	G	3440	0	3485	55	0
2	B	1646	0	1637	18	0
2	E	1646	0	1637	17	0
2	H	1658	0	1646	16	0
3	C	1622	0	1589	19	0
3	F	1618	0	1586	18	0
3	I	1637	0	1599	25	0
4	A	14	0	13	1	0
4	D	14	0	13	0	0
4	G	14	0	13	1	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
5	G	1	0	0	0	0
6	C	14	0	20	0	0
6	F	14	0	20	0	0
6	I	14	0	20	1	0
All	All	20286	0	20293	274	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 7.

All (274) 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)
3:I:8:PRO:O	3:I:102:THR:HG23	1.61	1.01
3:F:103:LYS:NZ	3:F:173:TYR:OH	2.02	0.93
1:A:176:LYS:NZ	1:A:263:ASP:OD2	2.05	0.88
1:G:60:GLU:OE2	1:G:191:LYS:NZ	2.06	0.88
1:A:454:ASN:H	1:G:374:THR:HG21	1.42	0.84
1:D:246:PRO:HB3	1:D:283:GLN:HA	1.59	0.82
1:D:266:ILE:HG22	1:D:267:THR:H	1.45	0.81
1:D:427:LYS:NZ	1:D:448:ASP:OD2	2.13	0.80
1:A:171:LEU:O	1:A:191:LYS:NZ	2.16	0.78
3:I:197:THR:HG22	3:I:204:PRO:HB3	1.64	0.78
3:F:197:THR:HG22	3:F:204:PRO:HB3	1.68	0.76
1:A:407:ILE:HD11	1:A:457:TYR:HB3	1.69	0.74
1:A:62:SER:OG	1:A:200:ASP:OD1	2.06	0.72
1:A:402:VAL:HG11	1:G:373:LEU:HD23	1.72	0.71
3:I:146:VAL:HG22	3:I:196:VAL:HG22	1.72	0.71
1:D:266:ILE:HD11	1:D:305:LEU:HD22	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:GLN:NE2	1:A:306:TYR:O	2.25	0.70
1:A:206:ILE:HG22	1:A:212:CYS:HB2	1.72	0.69
1:A:64:ILE:HD13	1:A:204:LEU:HD13	1.75	0.69
2:B:152:VAL:HG22	2:B:198:VAL:HG22	1.75	0.69
1:A:37:CYS:SG	1:A:319:SER:OG	2.51	0.69
1:G:196:LYS:NZ	1:G:295:GLU:OE2	2.15	0.69
1:A:246:PRO:HB3	1:A:283:GLN:HA	1.75	0.68
3:F:142:ARG:NH1	3:F:163:VAL:HG21	2.08	0.68
1:D:336:ARG:NH1	1:D:383:ASN:OD1	2.26	0.68
1:D:62:SER:OG	1:D:200:ASP:OD1	2.12	0.67
1:A:167:ILE:HG23	1:A:189:THR:HG21	1.77	0.67
3:I:27(A):ILE:HG23	3:I:68:GLY:HA2	1.77	0.66
1:D:392:ASP:OD2	1:D:493:SER:OG	2.13	0.66
1:A:374:THR:HG21	1:D:454:ASN:H	1.59	0.66
1:D:266:ILE:HG22	1:D:267:THR:N	2.11	0.66
1:D:167:ILE:HG23	1:D:189:THR:HG21	1.77	0.65
1:D:312:PRO:HG2	1:D:344:ASP:OD2	1.95	0.65
2:E:168:ALA:HB2	2:E:178:LEU:HD23	1.79	0.65
1:G:426:ASN:ND2	1:G:446:GLY:O	2.24	0.64
1:D:487:GLU:HA	1:G:486:ASP:OD2	1.97	0.64
1:D:206:ILE:HG22	1:D:212:CYS:HB2	1.79	0.63
1:A:156:LYS:NZ	1:D:462:GLN:HB3	2.13	0.63
1:A:36:THR:OG1	1:A:38:SER:OG	2.14	0.63
1:A:406:VAL:HG13	1:G:144:VAL:HB	1.79	0.63
1:G:246:PRO:HB3	1:G:283:GLN:HA	1.80	0.63
1:D:85:LYS:NZ	1:G:225:GLN:OE1	2.30	0.62
1:G:336:ARG:HH12	1:G:383:ASN:HA	1.64	0.62
3:I:37:GLN:HB2	3:I:47:LEU:HD11	1.81	0.61
3:F:4:LEU:HD11	3:F:90:SER:HB3	1.82	0.61
2:B:142:VAL:HG11	2:B:150:VAL:HG11	1.83	0.61
1:D:260:LEU:HD13	1:D:303:LEU:HD11	1.84	0.60
1:A:462:GLN:HA	1:G:156:LYS:HE2	1.84	0.60
3:F:37:GLN:HB2	3:F:47:LEU:HD11	1.84	0.60
3:I:103:LYS:NZ	3:I:173:TYR:OH	2.29	0.60
1:A:225:GLN:OE1	1:G:85:LYS:NZ	2.35	0.59
1:G:37:CYS:SG	1:G:319:SER:OG	2.60	0.59
1:D:385:ASP:O	1:D:388:ASN:ND2	2.27	0.59
1:D:267:THR:HB	1:D:270:GLN:HG3	1.85	0.58
3:I:142:ARG:NH2	3:I:163:VAL:HG21	2.18	0.58
1:A:487:GLU:HA	1:D:486:ASP:OD2	2.03	0.58
1:G:336:ARG:NH1	1:G:383:ASN:HA	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:119:PRO:HB3	2:B:145:TYR:HB3	1.86	0.57
1:G:395:ILE:HD13	1:G:492:ILE:HD13	1.87	0.56
2:E:168:ALA:HA	2:E:178:LEU:HB3	1.87	0.56
1:G:36:THR:OG1	1:G:38:SER:OG	2.18	0.56
1:A:159:HIS:CG	1:A:291:ILE:HD11	2.40	0.56
3:C:197:THR:HG22	3:C:204:PRO:HB3	1.87	0.56
1:A:449:THR:HB	1:A:456:LEU:HD11	1.87	0.56
1:D:270:GLN:HG2	1:D:309:ILE:HD12	1.86	0.56
1:A:486:ASP:OD2	1:G:487:GLU:HB3	2.06	0.56
1:G:321:LEU:HD21	1:G:473:PRO:HB3	1.86	0.56
1:A:79:ILE:HD12	1:A:214:ILE:HD13	1.88	0.56
1:G:336:ARG:HG2	1:G:394:LYS:O	2.07	0.55
2:H:168:ALA:HB2	2:H:178:LEU:HD23	1.88	0.55
2:E:200:HIS:ND1	2:E:203:SER:OG	2.39	0.55
2:E:82(B):ARG:HH11	2:E:82(B):ARG:HG3	1.72	0.55
1:A:379:VAL:HG22	1:A:391:TYR:CZ	2.42	0.55
2:E:119:PRO:HB3	2:E:145:TYR:HB3	1.88	0.55
3:F:46:LEU:HD21	3:F:49:PHE:HB3	1.88	0.55
1:G:28:ILE:HG22	1:G:410:LEU:HD11	1.89	0.55
2:B:18:VAL:HG12	2:B:82(C):LEU:HD11	1.90	0.54
1:D:266:ILE:CD1	1:D:305:LEU:HD22	2.36	0.54
2:B:168:ALA:HA	2:B:178:LEU:HB3	1.89	0.54
1:A:486:ASP:OD2	1:G:490:ALA:HB2	2.08	0.53
3:I:124:GLN:HG2	3:I:129:THR:O	2.08	0.53
1:D:266:ILE:HD11	1:D:305:LEU:CD2	2.38	0.53
1:A:479:ASP:HB3	1:A:481:LEU:HD13	1.89	0.53
1:A:49:ARG:NH1	1:A:52:TRP:CE2	2.76	0.53
1:G:216:ASN:HB3	1:G:218:GLU:OE1	2.08	0.53
3:I:46:LEU:HD21	3:I:49:PHE:HB3	1.90	0.52
1:A:318:THR:O	1:A:339:ARG:NH1	2.42	0.52
1:D:64:ILE:HD12	1:D:204:LEU:HD13	1.91	0.52
1:G:49:ARG:NH1	1:G:52:TRP:CE2	2.78	0.52
1:D:216:ASN:HB3	1:D:218:GLU:OE2	2.10	0.52
1:A:444:ASN:ND2	1:A:462:GLN:O	2.42	0.52
2:E:97:VAL:HG22	2:E:100(F):ILE:HD12	1.92	0.52
1:G:45:LEU:HD22	1:G:310:ASP:HA	1.91	0.52
1:A:260:LEU:O	1:A:264:MET:HG3	2.10	0.51
1:G:62:SER:HB2	1:G:200:ASP:OD1	2.10	0.51
1:A:196:LYS:NZ	1:A:295:GLU:OE1	2.43	0.51
1:A:423:THR:HG22	1:A:434:THR:HG23	1.93	0.51
3:C:186:TYR:HA	3:C:192:TYR:OH	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:ILE:O	1:A:503:LEU:N	2.39	0.51
2:E:68:THR:HB	2:E:81:GLU:HB3	1.93	0.50
1:A:216:ASN:HB3	1:A:218:GLU:OE1	2.10	0.50
1:A:318:THR:OG1	1:A:339:ARG:NH1	2.44	0.50
2:B:143:LYS:NZ	2:B:171:GLN:OE1	2.44	0.50
3:C:108:ARG:HG2	3:C:109:THR:N	2.26	0.50
3:F:30:ARG:HG2	3:F:51:ALA:CB	2.42	0.50
2:H:100(F):ILE:HD13	3:I:46:LEU:HD22	1.93	0.50
2:B:143:LYS:HE3	2:B:144:ASP:OD2	2.11	0.50
1:D:504:ALA:O	1:D:508:LYS:HG2	2.11	0.50
1:D:171:LEU:HD13	1:D:191:LYS:HB2	1.94	0.50
3:F:184:ALA:O	3:F:188:LYS:HG3	2.12	0.50
2:H:14:PRO:HD2	2:H:113:SER:HB3	1.94	0.50
1:A:159:HIS:ND1	1:A:291:ILE:HD11	2.27	0.50
3:C:30:ARG:HG2	3:C:51:ALA:CB	2.42	0.50
1:D:405:SER:HB2	1:D:452:VAL:HG21	1.94	0.50
1:D:336:ARG:NH2	1:D:338:ASP:OD2	2.37	0.50
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.94	0.49
1:A:59:ILE:HG23	1:A:193:LEU:HB3	1.94	0.49
1:G:68:LYS:HD2	4:G:601:NAG:H61	1.94	0.49
2:B:35:HIS:ND1	2:B:50:GLY:HA3	2.28	0.49
3:C:35:TRP:CD2	3:C:73:LEU:HB2	2.47	0.49
1:D:237:PHE:HD1	1:D:242:GLY:HA2	1.77	0.49
3:C:37:GLN:OE1	3:C:45:ARG:NH1	2.46	0.49
1:G:482:VAL:HB	1:G:502:SER:HB3	1.93	0.49
1:A:406:VAL:O	1:A:413:ILE:N	2.40	0.49
1:D:266:ILE:CG2	1:D:267:THR:H	2.22	0.49
1:D:416:CYS:O	1:D:437:ASN:HA	2.12	0.48
1:D:202:GLN:OE1	2:E:100(A):GLU:HB2	2.13	0.48
3:I:2:ILE:HD13	3:I:28:VAL:HG12	1.94	0.48
2:B:4:LEU:O	2:B:104:GLY:HA2	2.13	0.48
3:I:33:LEU:HD13	3:I:71:PHE:CD1	2.48	0.48
1:D:155:CYS:HA	1:D:158:LEU:HD23	1.95	0.48
2:E:1:GLN:OE1	2:E:1:GLN:N	2.43	0.48
3:F:61:ARG:NE	3:F:82:ASP:OD2	2.44	0.48
3:I:32:HIS:HB3	3:I:91:SER:OG	2.13	0.48
1:A:163:GLU:OE1	1:A:182:SER:OG	2.26	0.48
1:A:171:LEU:HD11	1:A:189:THR:HG22	1.95	0.48
1:G:341:TRP:HB2	1:G:352:PHE:HB2	1.95	0.48
1:A:156:LYS:NZ	1:D:462:GLN:HA	2.29	0.48
1:A:425:SER:HB2	1:A:449:THR:OG1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:30:ARG:HG2	3:C:51:ALA:HB2	1.95	0.48
2:H:119:PRO:HD2	2:H:205:THR:HG21	1.96	0.48
1:D:209:LYS:HE3	2:E:98:THR:CG2	2.44	0.48
3:I:210:ASN:HB2	3:I:214:GLU:HG2	1.95	0.48
1:A:153:ALA:O	1:A:157:VAL:HG23	2.14	0.47
1:A:400:THR:HA	1:G:394:LYS:NZ	2.28	0.47
1:G:321:LEU:HG	1:G:475:ILE:HD13	1.94	0.47
1:A:277:ASN:O	1:A:281:VAL:HG23	2.14	0.47
1:G:171:LEU:HD13	1:G:191:LYS:HB2	1.97	0.47
1:A:68:LYS:HD3	4:A:601:NAG:H61	1.96	0.47
1:A:206:ILE:HD11	2:B:100:THR:OG1	2.13	0.47
1:A:171:LEU:HD13	1:A:191:LYS:HB2	1.96	0.47
1:D:206:ILE:HD12	2:E:100(D):LEU:HA	1.95	0.47
1:G:79:ILE:HD11	1:G:220:VAL:HA	1.96	0.47
2:E:47:TRP:CZ2	2:E:49:GLY:HA2	2.50	0.47
1:G:381:LEU:HD21	1:G:390:LYS:HD2	1.97	0.47
1:A:252:LEU:HD21	1:A:260:LEU:HD12	1.97	0.47
1:A:62:SER:N	1:A:86:TYR:OH	2.48	0.47
1:D:54:THR:HG21	1:D:154:VAL:HG21	1.95	0.47
1:D:425:SER:HA	1:D:431:ILE:HA	1.97	0.47
3:F:124:GLN:O	3:F:127:SER:OG	2.31	0.47
1:G:138:LEU:HB3	1:G:141:LEU:HD12	1.97	0.47
2:B:168:ALA:HB2	2:B:178:LEU:HD23	1.96	0.47
3:F:32:HIS:HB3	3:F:91:SER:OG	2.14	0.47
3:F:30:ARG:HG2	3:F:51:ALA:HB2	1.96	0.47
2:H:35:HIS:HA	2:H:50:GLY:HA3	1.97	0.46
1:D:280:ILE:HG21	1:D:366:PHE:CG	2.50	0.46
1:G:240:ASN:HB3	1:G:243:VAL:O	2.15	0.46
1:A:318:THR:HG23	1:A:339:ARG:HB3	1.97	0.46
1:D:92:GLU:HG2	1:G:254:ASN:HD22	1.81	0.46
3:C:82:ASP:O	3:C:86:TYR:OH	2.19	0.46
2:B:124:LEU:HB3	3:C:118:PHE:CD2	2.50	0.46
1:D:171:LEU:O	1:D:191:LYS:NZ	2.30	0.46
1:A:498:LYS:HA	1:A:501:GLN:HG2	1.98	0.46
2:H:33:SER:O	2:H:94:THR:HA	2.16	0.46
1:A:239:VAL:HG13	1:D:246:PRO:HG2	1.98	0.46
1:D:352:PHE:CE2	1:D:367:CYS:HB3	2.51	0.46
1:G:83:LEU:O	1:G:87:LYS:HG3	2.16	0.46
2:H:96:GLY:O	2:H:100(F):ILE:HG13	2.16	0.45
3:I:108:ARG:HG2	3:I:109:THR:N	2.32	0.45
1:G:33:TYR:CE1	1:G:383:ASN:HB3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:LEU:O	1:D:264:MET:HG3	2.16	0.45
1:D:373:LEU:HD13	1:G:402:VAL:HG11	1.97	0.45
1:A:405:SER:HB3	1:A:457:TYR:CZ	2.52	0.45
3:C:35:TRP:CE2	3:C:73:LEU:HB2	2.52	0.45
3:I:106:PHE:HB2	3:I:166:GLN:NE2	2.32	0.45
1:A:156:LYS:HZ2	1:D:462:GLN:HB3	1.78	0.45
2:B:24:ILE:HB	2:B:76:ASP:HB3	1.99	0.45
1:A:379:VAL:HG22	1:A:391:TYR:CE2	2.52	0.44
1:A:400:THR:HA	1:G:394:LYS:HZ1	1.81	0.44
1:G:504:ALA:O	1:G:508:LYS:HD3	2.16	0.44
1:A:76:VAL:HA	1:A:214:ILE:HD12	1.98	0.44
1:A:188:LEU:HD12	1:A:188:LEU:HA	1.85	0.44
1:D:27:ASN:HB3	1:D:28:ILE:H	1.64	0.44
1:D:36:THR:OG1	1:D:38:SER:OG	2.29	0.44
1:A:505:PHE:CZ	1:D:505:PHE:HB3	2.53	0.44
2:E:122:PHE:CE2	3:F:124:GLN:HG3	2.53	0.44
1:A:211:SER:HB3	3:C:56:THR:H	1.82	0.44
1:A:156:LYS:HZ2	1:D:462:GLN:HA	1.81	0.44
1:G:64:ILE:HG21	1:G:204:LEU:HD13	2.00	0.44
3:C:132:VAL:HB	3:C:179:LEU:HB3	2.00	0.44
3:C:148:TRP:HB2	3:C:155:GLN:HB2	2.00	0.44
3:F:108:ARG:HD2	3:F:170:ASP:O	2.18	0.44
3:I:15:PRO:HG3	3:I:83:PHE:CE2	2.53	0.44
3:I:54:ARG:HG2	3:I:58:ILE:HB	1.99	0.44
1:D:171:LEU:HD11	1:D:189:THR:HG22	1.99	0.43
1:D:266:ILE:HG22	1:D:270:GLN:HB2	1.99	0.43
2:E:12:LYS:HG3	2:E:18:VAL:HB	2.00	0.43
2:H:68:THR:HB	2:H:81:GLU:HB3	2.00	0.43
1:D:270:GLN:NE2	1:D:306:TYR:O	2.52	0.43
3:I:191:VAL:HG22	3:I:210:ASN:OD1	2.19	0.43
1:A:78:LEU:HD13	1:A:220:VAL:HG11	2.00	0.43
1:A:400:THR:HG23	1:G:394:LYS:HE3	1.99	0.43
2:E:36:TRP:CD1	2:E:80:MET:HB3	2.53	0.43
2:H:123:PRO:HD3	2:H:209:LYS:HE2	2.01	0.43
3:C:33:LEU:HD22	3:C:71:PHE:CD2	2.52	0.43
1:D:267:THR:O	1:D:271:LYS:HG3	2.19	0.43
1:D:142:LEU:HD23	1:D:373:LEU:HG	2.01	0.43
2:H:166:PHE:CE2	3:I:176:SER:HB3	2.53	0.43
2:E:36:TRP:NE1	2:E:80:MET:HB3	2.34	0.43
3:I:140:TYR:CG	3:I:141:PRO:HA	2.54	0.43
1:A:33:TYR:OH	1:A:383:ASN:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:SER:OG	1:A:363:ASN:N	2.52	0.42
1:G:213:SER:HB2	3:I:53:SER:OG	2.19	0.42
3:C:167:ASP:HB3	3:C:170:ASP:OD1	2.18	0.42
2:E:35:HIS:O	2:E:92:CYS:HA	2.19	0.42
3:C:83:PHE:CD1	3:C:104:VAL:HG12	2.55	0.42
1:G:146:SER:HB3	1:G:149:ALA:HB2	2.00	0.42
2:H:151:THR:OG1	2:H:199:ASN:HB3	2.20	0.42
2:B:47:TRP:CD2	3:C:96:PHE:HB2	2.54	0.42
1:D:190:PHE:CE1	1:D:260:LEU:HG	2.55	0.42
1:A:338:ASP:N	1:A:338:ASP:OD1	2.53	0.42
2:B:97:VAL:HG22	2:B:100(F):ILE:HD12	2.01	0.42
2:H:12:LYS:HE3	2:H:18:VAL:HA	2.01	0.42
3:I:89:LEU:HD11	3:I:96:PHE:HB3	2.02	0.42
3:F:54:ARG:HD2	3:F:58:ILE:O	2.20	0.42
1:G:379:VAL:HG23	1:G:391:TYR:CD1	2.55	0.42
1:A:375:LEU:HB3	1:A:379:VAL:HG21	2.02	0.42
1:D:69:CYS:N	1:D:207:LEU:O	2.53	0.41
1:D:49:ARG:NH1	1:D:52:TRP:CE2	2.87	0.41
1:G:483:PHE:HD1	1:G:499:ILE:HD11	1.85	0.41
1:A:201:LYS:NZ	1:A:202:GLN:HE21	2.19	0.41
1:G:206:ILE:HG22	1:G:212:CYS:HB2	2.02	0.41
6:I:302:PEG:H41	6:I:302:PEG:H22	1.91	0.41
3:I:54:ARG:NH1	3:I:62:PHE:O	2.44	0.41
1:A:316:LEU:HD23	1:A:338:ASP:O	2.21	0.41
2:B:101:ASP:OD2	3:C:46:LEU:HB3	2.20	0.41
1:A:427:LYS:HG2	1:A:448:ASP:OD2	2.21	0.41
3:C:81:GLU:OE1	3:C:81:GLU:N	2.36	0.41
1:D:415:SER:HB3	1:D:417:TYR:CE2	2.55	0.41
3:F:107:LYS:HA	3:F:140:TYR:OH	2.21	0.41
1:G:49:ARG:HD2	1:G:52:TRP:CH2	2.56	0.41
2:H:168:ALA:HA	2:H:178:LEU:HB3	2.01	0.41
2:H:36:TRP:CE2	2:H:80:MET:HB3	2.55	0.41
1:A:414:VAL:O	1:A:439:CYS:HA	2.20	0.41
2:B:59:TYR:HE1	2:B:69:VAL:HG23	1.85	0.41
1:G:293:LYS:HG2	1:G:294:GLU:HG3	2.02	0.41
1:A:422:CYS:HB3	1:A:452:VAL:HG22	2.03	0.41
2:B:66:ARG:HD2	2:B:82(A):GLY:O	2.20	0.41
1:G:73:ASP:OD1	1:G:74:ALA:N	2.54	0.41
1:A:148:ILE:HB	1:A:288:ILE:HD11	2.03	0.41
1:A:458:TYR:CD2	1:G:150:SER:HB3	2.55	0.41
3:F:194:CYS:O	3:F:206:THR:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:210:GLN:N	2:H:100(G):ASP:OD1	2.45	0.41
1:A:204:LEU:N	1:A:205:PRO:HD2	2.35	0.41
1:G:379:VAL:HG23	1:G:391:TYR:CG	2.56	0.41
1:A:328:GLU:OE2	1:G:391:TYR:HA	2.21	0.41
1:A:235:ARG:CZ	1:A:235:ARG:HB2	2.51	0.40
1:A:426:ASN:OD1	1:A:427:LYS:N	2.54	0.40
1:D:237:PHE:CD1	1:D:242:GLY:HA2	2.56	0.40
1:A:281:VAL:O	1:A:285:SER:OG	2.28	0.40
1:A:310:ASP:OD1	1:A:364:ARG:NH1	2.53	0.40
1:A:36:THR:HG21	1:A:386:ILE:CD1	2.51	0.40
3:F:35:TRP:CE2	3:F:73:LEU:HB2	2.57	0.40
3:I:30:ARG:HG2	3:I:51:ALA:CB	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	441/568 (78%)	410 (93%)	30 (7%)	1 (0%)	47	81
1	D	445/568 (78%)	424 (95%)	21 (5%)	0	100	100
1	G	440/568 (78%)	417 (95%)	23 (5%)	0	100	100
2	B	217/228 (95%)	210 (97%)	7 (3%)	0	100	100
2	E	217/228 (95%)	211 (97%)	6 (3%)	0	100	100
2	H	219/228 (96%)	207 (94%)	12 (6%)	0	100	100
3	C	211/215 (98%)	203 (96%)	8 (4%)	0	100	100
3	F	210/215 (98%)	203 (97%)	7 (3%)	0	100	100
3	I	213/215 (99%)	205 (96%)	7 (3%)	1 (0%)	29	68
All	All	2613/3033 (86%)	2490 (95%)	121 (5%)	2 (0%)	51	84

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	389	PRO
3	I	68	GLY

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	406/510 (80%)	404 (100%)	2 (0%)	88	94
1	D	410/510 (80%)	409 (100%)	1 (0%)	93	98
1	G	405/510 (79%)	402 (99%)	3 (1%)	84	93
2	B	184/191 (96%)	184 (100%)	0	100	100
2	E	184/191 (96%)	184 (100%)	0	100	100
2	H	186/191 (97%)	186 (100%)	0	100	100
3	C	183/185 (99%)	183 (100%)	0	100	100
3	F	183/185 (99%)	183 (100%)	0	100	100
3	I	185/185 (100%)	184 (100%)	1 (0%)	88	94
All	All	2326/2658 (88%)	2319 (100%)	7 (0%)	92	97

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

Mol	Chain	Res	Type
1	A	190	PHE
1	A	213	SER
1	D	213	SER
1	G	213	SER
1	G	343	CYS
1	G	381	LEU
3	I	52	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 3 are monoatomic - leaving 9 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	$\# Z > 2$
6	PEG	C	301	-	6,6,6	0.49	0	5,5,5	0.29	0
6	PEG	I	301	-	6,6,6	0.51	0	5,5,5	0.28	0
4	NAG	A	601	1	14,14,15	0.41	0	17,19,21	0.43	0
4	NAG	D	601	1	14,14,15	0.60	0	17,19,21	0.60	1 (5%)
4	NAG	G	601	1	14,14,15	0.52	0	17,19,21	0.42	0
6	PEG	F	301	-	6,6,6	0.49	0	5,5,5	0.25	0
6	PEG	F	302	-	6,6,6	0.50	0	5,5,5	0.25	0
6	PEG	C	302	-	6,6,6	0.49	0	5,5,5	0.22	0
6	PEG	I	302	-	6,6,6	0.48	0	5,5,5	0.28	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
6	PEG	C	301	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PEG	I	301	-	-	1/4/4/4	-
4	NAG	A	601	1	-	2/6/23/26	0/1/1/1
4	NAG	D	601	1	-	2/6/23/26	0/1/1/1
4	NAG	G	601	1	-	2/6/23/26	0/1/1/1
6	PEG	F	301	-	-	2/4/4/4	-
6	PEG	F	302	-	-	2/4/4/4	-
6	PEG	C	302	-	-	1/4/4/4	-
6	PEG	I	302	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	601	NAG	C1-O5-C5	2.01	114.92	112.19

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	601	NAG	O5-C5-C6-O6
4	A	601	NAG	O5-C5-C6-O6
4	G	601	NAG	O5-C5-C6-O6
4	D	601	NAG	C4-C5-C6-O6
4	G	601	NAG	C4-C5-C6-O6
4	A	601	NAG	C4-C5-C6-O6
6	F	302	PEG	O2-C3-C4-O4
6	F	302	PEG	O1-C1-C2-O2
6	I	302	PEG	O2-C3-C4-O4
6	C	301	PEG	O2-C3-C4-O4
6	F	301	PEG	O1-C1-C2-O2
6	C	302	PEG	C1-C2-O2-C3
6	I	301	PEG	C1-C2-O2-C3
6	C	301	PEG	C1-C2-O2-C3
6	F	301	PEG	O2-C3-C4-O4
6	C	301	PEG	C4-C3-O2-C2
6	I	302	PEG	C4-C3-O2-C2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	601	NAG	1	0
4	G	601	NAG	1	0
6	I	302	PEG	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, 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	445/568 (78%)	-0.32	2 (0%) 92 90	21, 80, 134, 209	0
1	D	449/568 (79%)	-0.26	2 (0%) 92 90	20, 87, 141, 191	0
1	G	444/568 (78%)	-0.15	3 (0%) 87 83	19, 96, 142, 174	0
2	B	221/228 (96%)	-0.47	0 100 100	23, 46, 89, 127	0
2	E	221/228 (96%)	-0.48	1 (0%) 91 88	23, 42, 79, 137	0
2	H	223/228 (97%)	-0.56	1 (0%) 92 90	21, 44, 82, 114	0
3	C	213/215 (99%)	-0.63	0 100 100	21, 35, 61, 98	0
3	F	212/215 (98%)	-0.58	0 100 100	20, 41, 78, 113	0
3	I	215/215 (100%)	-0.65	0 100 100	15, 28, 63, 94	0
All	All	2643/3033 (87%)	-0.40	9 (0%) 94 91	15, 57, 130, 209	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	133	GLY	3.2
1	G	36	THR	2.9
1	G	39	ALA	2.4
1	A	504	ALA	2.4
2	E	133	GLY	2.4
1	D	490	ALA	2.2
1	G	505	PHE	2.1
1	D	485	SER	2.1
1	A	507	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates [i](#)

There are no monosaccharides 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	NAG	G	601	14/15	0.87	0.30	46,55,59,59	0
4	NAG	A	601	14/15	0.88	0.39	43,55,63,64	0
6	PEG	C	302	7/7	0.89	0.27	28,34,39,39	0
6	PEG	F	302	7/7	0.91	0.16	8,10,12,14	0
6	PEG	F	301	7/7	0.91	0.20	14,15,17,18	0
4	NAG	D	601	14/15	0.92	0.31	46,53,64,65	0
6	PEG	I	301	7/7	0.92	0.19	3,12,21,23	0
6	PEG	I	302	7/7	0.92	0.18	27,31,35,36	0
5	CD	A	602	1/1	0.94	0.12	135,135,135,135	0
6	PEG	C	301	7/7	0.94	0.18	16,17,21,24	0
5	CD	G	602	1/1	0.96	0.06	76,76,76,76	0
5	CD	D	602	1/1	0.99	0.04	116,116,116,116	0

6.5 Other polymers [i](#)

There are no such residues in this entry.