Full wwPDB X-ray Structure Validation Report (i)

Oct 7, 2023 – 03:42 PM EDT

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 (i) 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 (i)) were used in the production of this report:

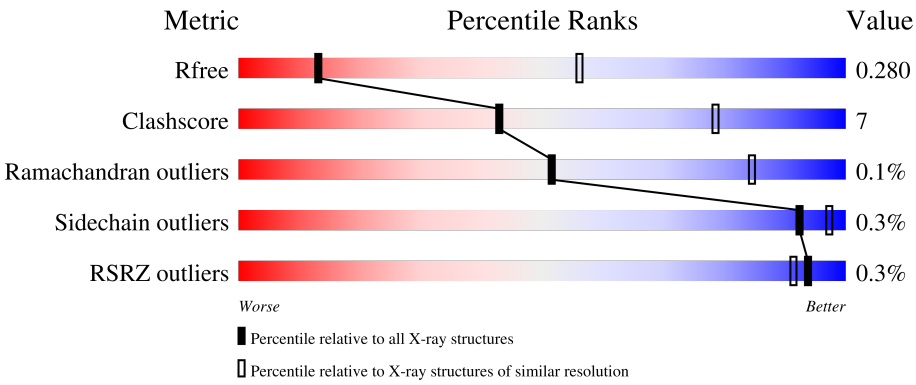
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.50 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 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 <=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	59% 19% 22%
1	D	568	66% 13% 21%
1	G	568	% 64% 13% 22%
2	B	228	84% 13% •
2	E	228	86% 11% •

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Mol	Chain	Length	Quality of chain
2	H	228	87% 11% •
3	C	215	85% 14% •
3	F	215	84% 15% •
3	I	215	79% 20%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	445	3449	2181	569	676	23	0	0	0
1	D	449	3483	2201	574	685	23	0	0	0
1	G	444	3440	2176	567	674	23	0	0	0

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

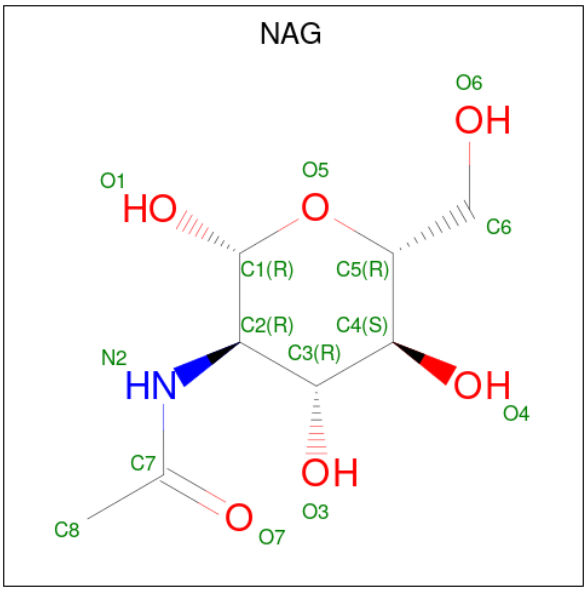
- Molecule 2 is a protein called Fab AM22 heavy chain.

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

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

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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

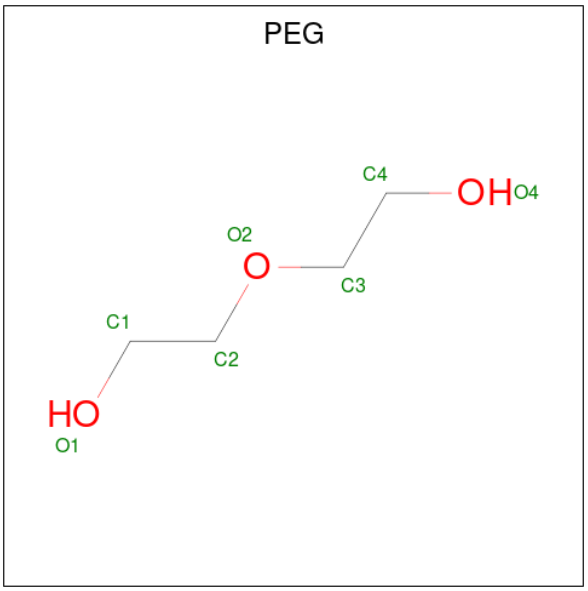


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	14	8	1	5	0	0
			Total	C	N	O		
4	D	1	14	8	1	5	0	0
			Total	C	N	O		
4	G	1	14	8	1	5	0	0

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

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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



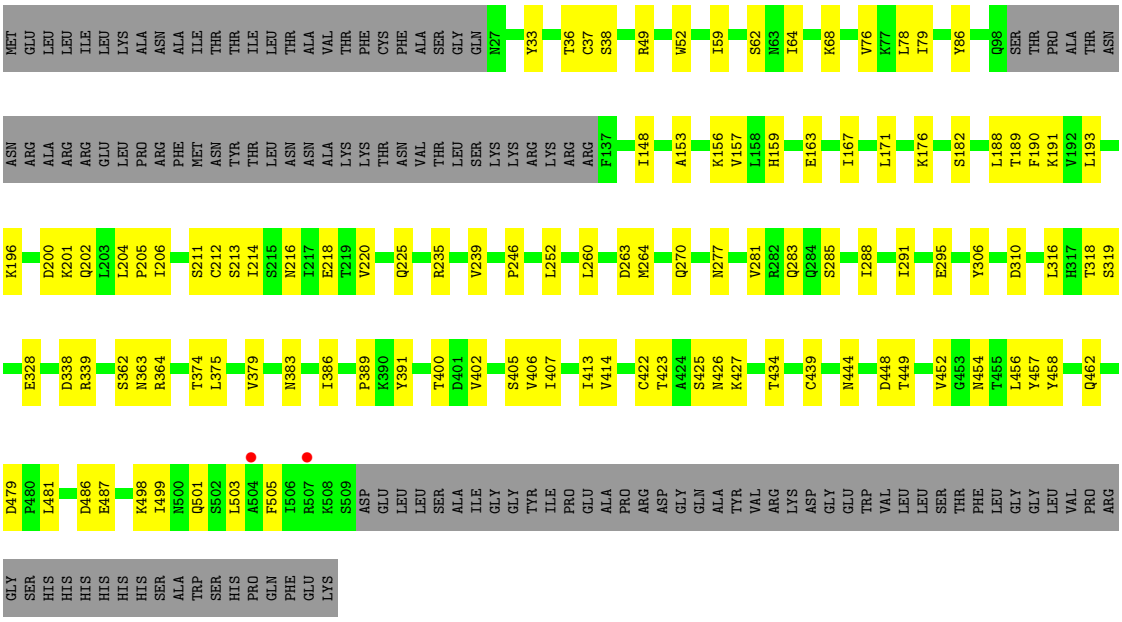
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
6	C	1	7	4	3		0	0
			Total	C	O			
6	C	1	7	4	3		0	0
			Total	C	O			
6	F	1	7	4	3		0	0
			Total	C	O			
6	F	1	7	4	3		0	0
			Total	C	O			
6	I	1	7	4	3		0	0
			Total	C	O			
6	I	1	7	4	3		0	0

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.

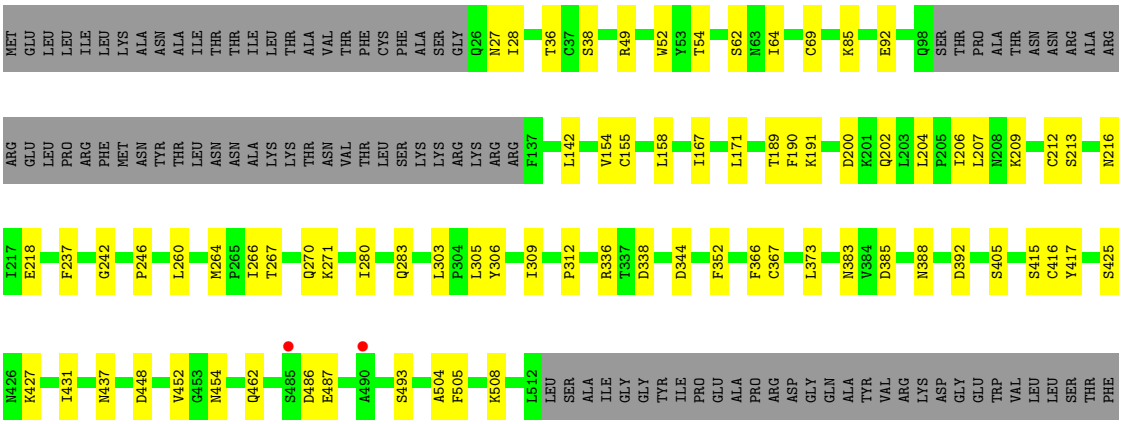
• Molecule 1: RSV fusion glycoprotein

Chain A: 59% 19% 22%



• Molecule 1: RSV fusion glycoprotein

Chain D: 66% 13% 21%



LEU GLY GLY LEU VAL PRO ARG GLY SER HIS HIS HIS HIS HIS HIS SER ALA TRP SER HIS PRO GLN PHE GLU LYS

- Molecule 1: RSV fusion glycoprotein

Chain G:

MET GLU LEU LEU ILE LEU LYS ALA ASN ALA ILE THR THR ILE LEU THR ALA VAL THR PHE CYS PHE ALA SER GLY GLN N27 I28 Y33 T36 C37 S38 A39 L45 R49 W52 E60 L61 S62 N63 I64 K68 D73 A74 I79 L83 D84 K85 Y86 K87

M97 GLN SER THR PRO ALA THR ASN ASN ARG ALA ARG ARG GLU LEU PRO ARG PHE MET ASN TYR THR LEU ASN ASN ALA LYS LYS THR ASN VAL THR LEU SER LYS LYS ARG LYS ARG ARG F137 L138 L141 V144 G145 S146 A149 S150 K156 L171 K191 K196

D200 L204 P205 I206 Q210 S211 C212 S213 N216 I217 E218 T219 V220 Q225 N240 V243 P246 N254 Q283 K293 E294 E295 D310 S319 P320 L321 R336 W341 Y342 C343 F352 L373 T374 V379 N380 L381 C382 N383 K390 Y391

K394 I395 V402 L410 N426 G446 P473 I474 I475 V482 F483 D486 E487 A490 S491 I492 I499 S502 L503 A504 F505 K508 S509 ASP GLU LEU LEU SER ALA ILE GLY GLY TYR ILE PRO GLU ALA PRO ARG ASP GLY GLN ALA TYR VAL ARG LYS ASP GLY

GLU TRP VAL LEU LEU SER THR PHE LEU GLY GLY LEU VAL PRO ARG GLY SER HIS HIS HIS HIS HIS SER ALA TRP SER HIS PRO GLN PHE GLU LYS

- Molecule 2: Fab AM22 heavy chain

Chain B:

Q1 L4 V18 I24 H35 W47 G50 Y59 R66 V69 D76 G82A R82B L82C V97 T100 I100F D100G D101 G104 P119 L124 S127 SER LYS SER THR SER G133 V142 K143 D144 Y145 V150 T151 V152 A168 Q171

L178 V198 S215 CYS ASP

- Molecule 2: Fab AM22 heavy chain

Chain E:

Q1 K12 V18 H35 W36 W47 M48 G49 T68 M80 E81 R82B C92 V97 T98 E100A L100D G100E I100F P119 F122 S127 SER LYS SER THR SER G133 Y145 A168 L178 H200 S203 S215 CYS ASP

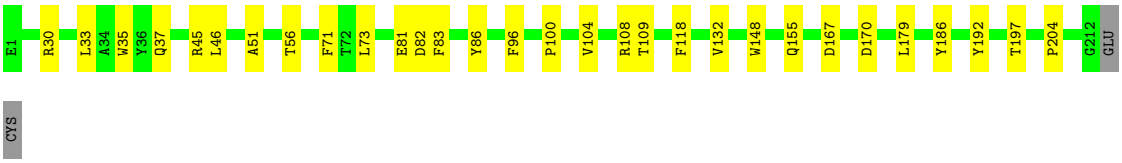
- Molecule 2: Fab AM22 heavy chain

Chain H:

Q1 K12 K13 P14 V18 S33 I34 H35 W36 G50 T68 M80 E81 T94 L95 G96 I100F D100G S113 P119 P123 S128 LYS SER THR SER G133 Y145 T151 F166 P167 A168 L178 N199 T205 K209 C216 ASP

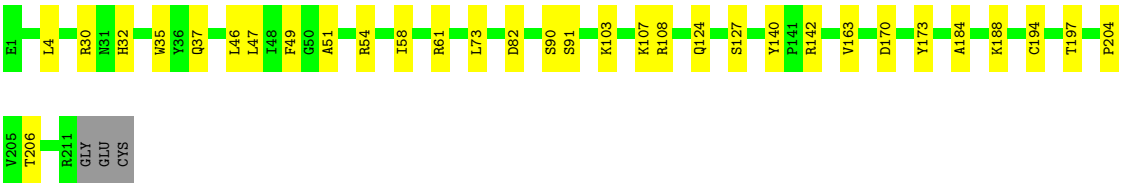
- Molecule 3: Fab AM22 light chain

Chain C:



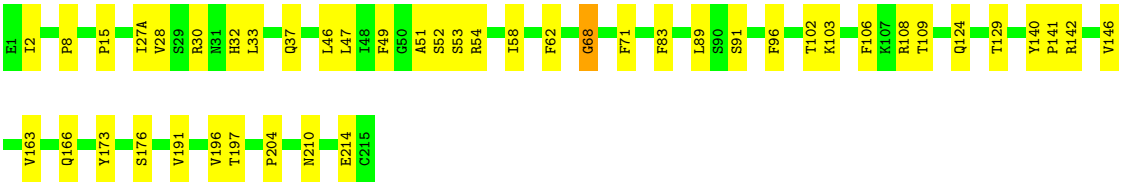
• Molecule 3: Fab AM22 light chain

Chain F:



• Molecule 3: Fab AM22 light chain

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 2 21	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
$< I/\sigma(I) >$ [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]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	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.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CD, PEG, NAG

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:64:ILE:HD13	1:A:204:LEU:HD13	1.75	0.69
1:A:206:ILE:HG22	1:A:212:CYS:HB2	1.72	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
1:G:36:THR:OG1	1:G:38:SER:OG	2.18	0.56
2:E:168:ALA:HA	2:E:178:LEU:HB3	1.87	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:HG3	2:E:82(B):ARG:HH11	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
1:D:504:ALA:O	1:D:508:LYS:HG2	2.11	0.50
2:B:143:LYS:HE3	2:B:144:ASP:OD2	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
1:D:405:SER:HB2	1:D:452:VAL:HG21	1.94	0.50
3:C:30:ARG:HG2	3:C:51:ALA:CB	2.42	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
1:G:482:VAL:HB	1:G:502:SER:HB3	1.93	0.49
3:C:37:GLN:OE1	3:C:45:ARG:NH1	2.46	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
1:A:62:SER:N	1:A:86:TYR:OH	2.48	0.47
1:A:252:LEU:HD21	1:A:260:LEU:HD12	1.97	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
1:G:138:LEU:HB3	1:G:141:LEU:HD12	1.97	0.47
1:G:381:LEU:HD21	1:G:390:LYS:HD2	1.97	0.47
2:E:47:TRP:CZ2	2:E:49:GLY:HA2	2.50	0.47
3:F:124:GLN:O	3:F:127:SER:OG	2.31	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:156:LYS:HZ2	1:D:462:GLN:HA	1.81	0.44
1:A:211:SER:HB3	3:C:56:THR:H	1.82	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
1:D:142:LEU:HD23	1:D:373:LEU:HG	2.01	0.43
1:D:267:THR:O	1:D:271:LYS:HG3	2.19	0.43
3:C:33:LEU:HD22	3:C:71:PHE:CD2	2.52	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
1:G:146:SER:HB3	1:G:149:ALA:HB2	2.00	0.42
3:C:83:PHE:CD1	3:C:104:VAL:HG12	2.55	0.42
2:H:151:THR:OG1	2:H:199:ASN:HB3	2.20	0.42
1:D:190:PHE:CE1	1:D:260:LEU:HG	2.55	0.42
2:B:47:TRP:CD2	3:C:96:PHE:HB2	2.54	0.42
1:A:338:ASP:OD1	1:A:338:ASP:N	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
1:G:379:VAL:HG23	1:G:391:TYR:CD1	2.55	0.42
3:F:54:ARG:HD2	3:F:58:ILE:O	2.20	0.42
1:A:375:LEU:HB3	1:A:379:VAL:HG21	2.02	0.42
1:D:49:ARG:NH1	1:D:52:TRP:CE2	2.87	0.41
1:D:69:CYS:N	1:D:207:LEU:O	2.53	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
3:I:54:ARG:NH1	3:I:62:PHE:O	2.44	0.41
6:I:302:PEG:H22	6:I:302:PEG:H41	1.91	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
1:D:415:SER:HB3	1:D:417:TYR:CE2	2.55	0.41
1:G:49:ARG:HD2	1:G:52:TRP:CH2	2.56	0.41
3:C:81:GLU:OE1	3:C:81:GLU:N	2.36	0.41
3:F:107:LYS:HA	3:F:140:TYR:OH	2.21	0.41
2:H:36:TRP:CE2	2:H:80:MET:HB3	2.55	0.41
2:H:168:ALA:HA	2:H:178:LEU:HB3	2.01	0.41
1:A:414:VAL:O	1:A:439:CYS:HA	2.20	0.41
1:G:293:LYS:HG2	1:G:294:GLU:HG3	2.02	0.41
2:B:59:TYR:HE1	2:B:69:VAL:HG23	1.85	0.41
1:A:422:CYS:HB3	1:A:452:VAL:HG22	2.03	0.41
1:G:73:ASP:OD1	1:G:74:ALA:N	2.54	0.41
2:B:66:ARG:HD2	2:B:82(A):GLY:O	2.20	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
1:G:210:GLN:N	2:H:100(G):ASP:OD1	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:194:CYS:O	3:F:206:THR:HA	2.21	0.41
1:A:204:LEU:N	1:A:205:PRO:HD2	2.35	0.41
1:A:328:GLU:OE2	1:G:391:TYR:HA	2.21	0.41
1:G:379:VAL:HG23	1:G:391:TYR:CG	2.56	0.41
1:A:235:ARG:HB2	1:A:235:ARG:CZ	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:36:THR:HG21	1:A:386:ILE:CD1	2.51	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
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 (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	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 (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	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

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

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
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	302	-	6,6,6	0.50	0	5,5,5	0.25	0
6	PEG	I	301	-	6,6,6	0.51	0	5,5,5	0.28	0
6	PEG	I	302	-	6,6,6	0.48	0	5,5,5	0.28	0
6	PEG	C	302	-	6,6,6	0.49	0	5,5,5	0.22	0
4	NAG	A	601	1	14,14,15	0.41	0	17,19,21	0.43	0
6	PEG	C	301	-	6,6,6	0.49	0	5,5,5	0.29	0
6	PEG	F	301	-	6,6,6	0.49	0	5,5,5	0.25	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	NAG	D	601	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	601	1	-	2/6/23/26	0/1/1/1
6	PEG	F	302	-	-	2/4/4/4	-
6	PEG	I	301	-	-	1/4/4/4	-
6	PEG	I	302	-	-	2/4/4/4	-
6	PEG	C	302	-	-	1/4/4/4	-
4	NAG	A	601	1	-	2/6/23/26	0/1/1/1
6	PEG	C	301	-	-	3/4/4/4	-
6	PEG	F	301	-	-	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(^{o})	Ideal(^{o})
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	A	601	NAG	C4-C5-C6-O6
4	G	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	G	601	NAG	1	0
6	I	302	PEG	1	0
4	A	601	NAG	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 (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	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 (i)

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	301	7/7	0.91	0.20	14,15,17,18	0
6	PEG	F	302	7/7	0.91	0.16	8,10,12,14	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
6	PEG	C	301	7/7	0.94	0.18	16,17,21,24	0
5	CD	A	602	1/1	0.94	0.12	135,135,135,135	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.