



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 12:48 PM EST

PDB ID : 5MDM
Title : Structural intermediates in the fusion associated transition of vesiculovirus glycoprotein
Authors : Baquero, E.; Albertini, A.A.; Gaudin, Y.; Bressanelli, S.
Deposited on : 2016-11-11
Resolution : 3.00 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

<http://wwpdb.org/validation/2016/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	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

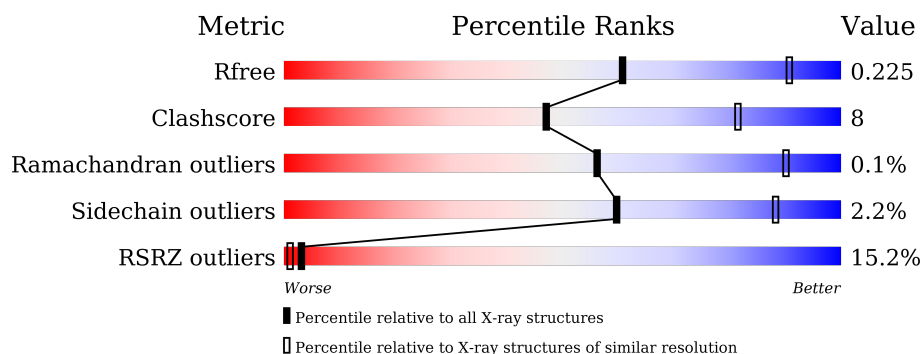
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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. 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	419	<div> <div>17%</div> <div>79%</div> <div>18%</div> <div>•</div> </div>
1	C	419	<div> <div>11%</div> <div>78%</div> <div>17%</div> <div>5%</div> </div>
1	E	419	<div> <div>19%</div> <div>77%</div> <div>21%</div> <div>•</div> </div>
1	F	419	<div> <div>12%</div> <div>77%</div> <div>18%</div> <div>5%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	E	501	-	-	-	X

2 Entry composition [i](#)

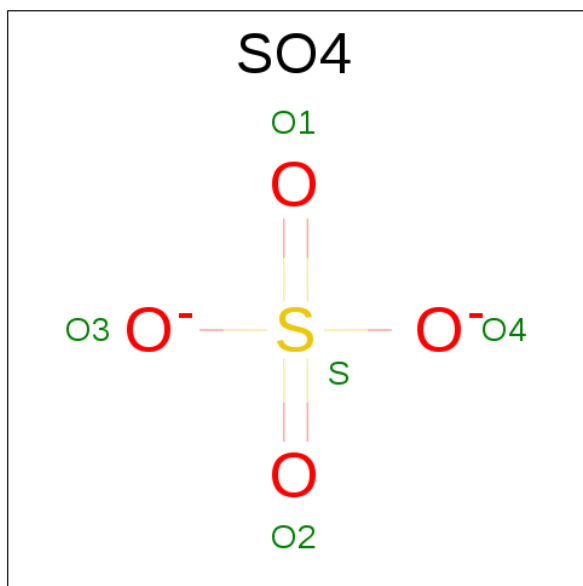
There are 4 unique types of molecules in this entry. The entry contains 12825 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	410	Total	C	N	O	S	0	0	0
			3223	2058	540	607	18			
1	F	398	Total	C	N	O	S	0	0	0
			3140	2009	526	587	18			
1	A	410	Total	C	N	O	S	0	0	0
			3223	2058	540	607	18			
1	C	398	Total	C	N	O	S	0	0	0
			3140	2009	526	587	18			

- Molecule 2 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



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

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: C₆H₁₂O₅).

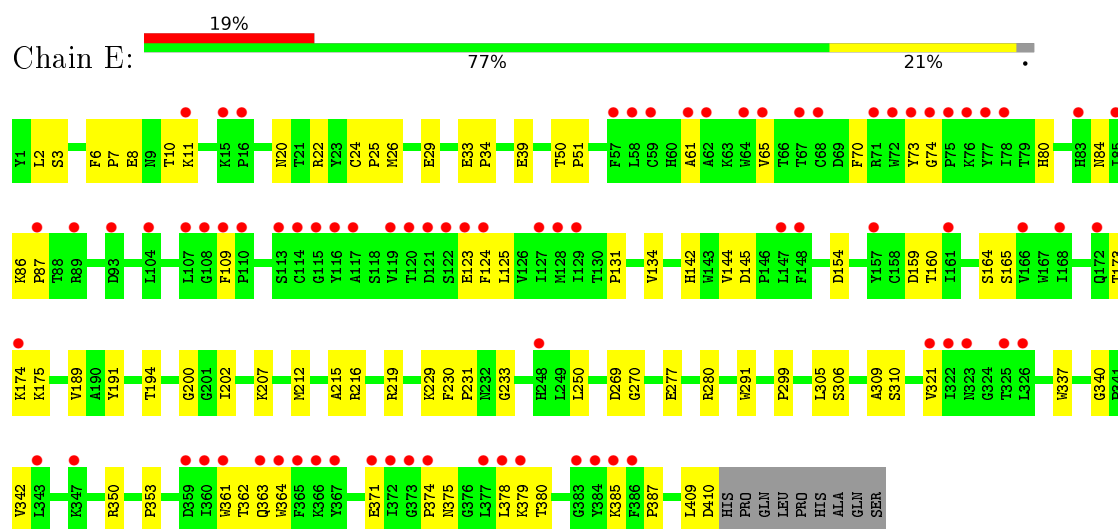


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	C	O	0	0
			10	6	4		

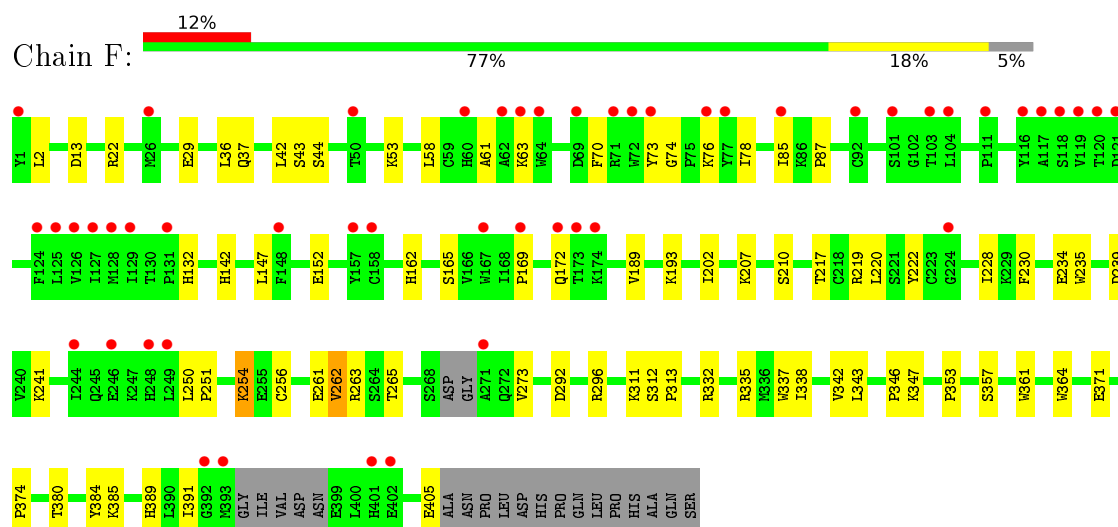
3 Residue-property plots

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

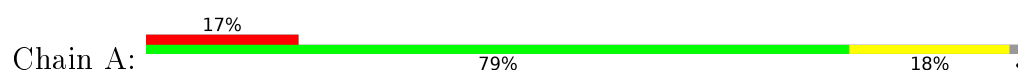
• Molecule 1: Glycoprotein

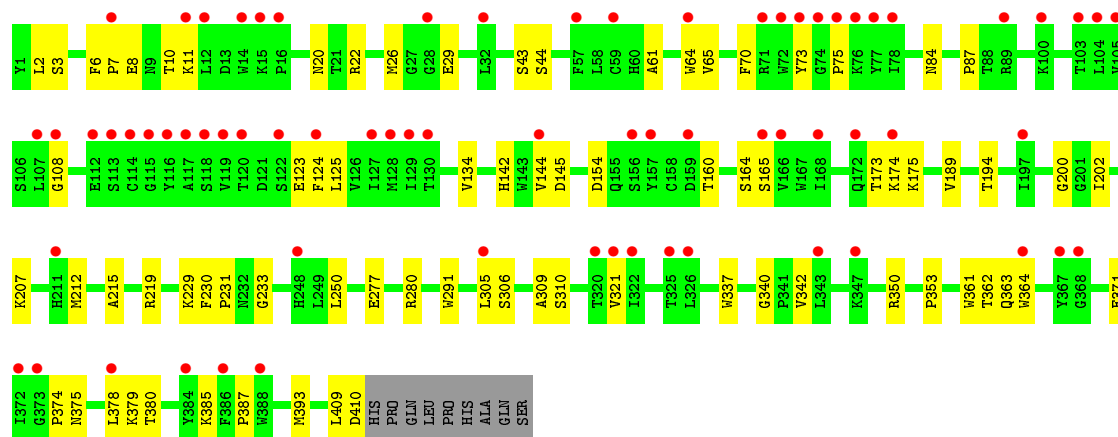


• Molecule 1: Glycoprotein

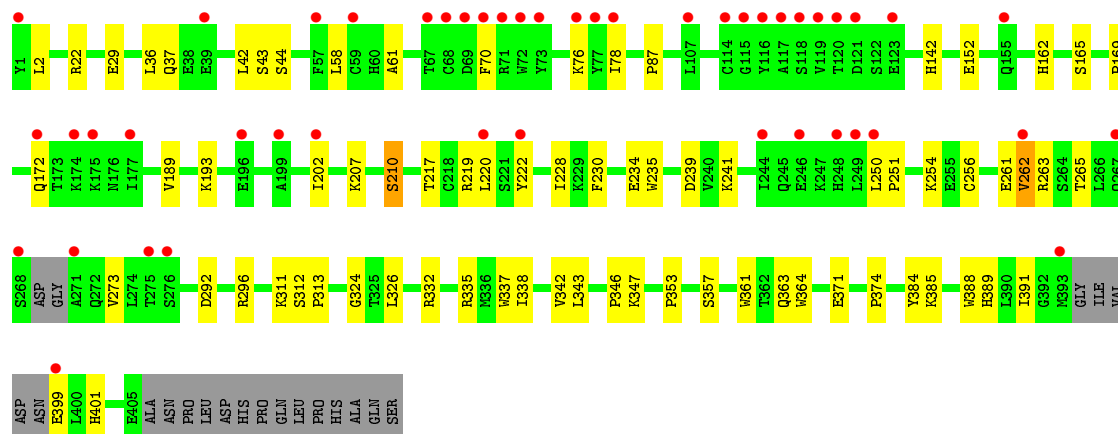
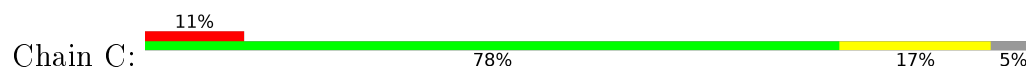


• Molecule 1: Glycoprotein





● Molecule 1: Glycoprotein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	150.34Å 228.21Å 78.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.11 – 3.00 49.11 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.11-3.00) 99.7 (49.11-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.188 , 0.222 0.192 , 0.225	Depositor DCC
R_{free} test set	2757 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	84.6	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 78.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12825	wwPDB-VP
Average B, all atoms (Å ²)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% 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: FUC, SO4, 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	0.28	0/3317	0.45	0/4510
1	C	0.27	0/3231	0.43	0/4388
1	E	0.28	0/3317	0.44	0/4510
1	F	0.26	0/3231	0.43	0/4388
All	All	0.27	0/13096	0.44	0/17796

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	3223	0	3127	48	2
1	C	3140	0	3052	52	0
1	E	3223	0	3128	52	2
1	F	3140	0	3050	55	0
2	E	5	0	0	0	0
3	A	14	0	13	0	0
3	C	14	0	13	0	0
3	F	56	0	49	1	0
4	F	10	0	10	0	0
All	All	12825	0	12442	190	2

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 8.

All (190) 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:212:MET:HG3	1:A:231:PRO:HD2	1.68	0.74
1:E:409:LEU:O	1:A:73:TYR:OH	2.04	0.74
1:E:212:MET:HG3	1:E:231:PRO:HD2	1.70	0.72
1:F:22:ARG:NH2	1:F:292:ASP:OD1	2.19	0.72
1:F:76:LYS:HD3	1:A:125:LEU:HD23	1.71	0.70
1:A:305:LEU:HD11	1:A:321:VAL:HG23	1.74	0.69
1:E:305:LEU:HD11	1:E:321:VAL:HG23	1.74	0.69
1:E:131:PRO:HB2	1:A:75:PRO:HB3	1.76	0.67
1:C:169:PRO:HG2	1:C:172:GLN:HG2	1.78	0.66
1:C:219:ARG:HG3	1:C:250:LEU:HD11	1.75	0.66
1:F:169:PRO:HG2	1:F:172:GLN:HG2	1.77	0.66
1:A:380:THR:OG1	1:A:385:LYS:NZ	2.30	0.65
1:C:22:ARG:NH2	1:C:292:ASP:OD1	2.22	0.64
1:F:219:ARG:HG3	1:F:250:LEU:HD11	1.78	0.64
1:C:361:TRP:CE2	1:C:374:PRO:HD3	2.33	0.64
1:E:125:LEU:HD23	1:C:76:LYS:HD3	1.79	0.64
1:E:380:THR:OG1	1:E:385:LYS:NZ	2.31	0.63
1:E:229:LYS:HE2	1:E:233:GLY:HA2	1.81	0.63
1:A:229:LYS:HE2	1:A:233:GLY:HA2	1.82	0.62
1:E:84:ASN:HB3	1:E:164:SER:HB3	1.82	0.62
1:F:361:TRP:CE2	1:F:374:PRO:HD3	2.34	0.61
1:E:123:GLU:HG3	1:C:78:ILE:HB	1.82	0.60
1:A:410:ASP:N	1:C:324:GLY:O	2.26	0.59
1:A:22:ARG:HG2	1:A:291:TRP:CG	2.38	0.58
1:E:22:ARG:HG2	1:E:291:TRP:CG	2.38	0.58
1:E:410:ASP:HB2	1:A:73:TYR:CE2	2.39	0.58
1:E:361:TRP:CE2	1:E:374:PRO:HD3	2.40	0.57
1:A:361:TRP:CE2	1:A:374:PRO:HD3	2.40	0.57
1:E:189:VAL:HG13	1:E:202:ILE:HG23	1.87	0.57
1:A:189:VAL:HG13	1:A:202:ILE:HG23	1.87	0.57
1:C:37:GLN:HG3	1:C:193:LYS:HD3	1.87	0.57
1:F:13:ASP:OD2	1:F:53:LYS:HD2	2.05	0.56
1:F:207:LYS:HA	1:F:335:ARG:HG3	1.87	0.56
1:A:61:ALA:HB2	1:A:87:PRO:HB3	1.87	0.56
1:F:78:ILE:HB	1:A:123:GLU:HG3	1.88	0.56
1:C:207:LYS:HA	1:C:335:ARG:HG3	1.88	0.56
1:E:364:TRP:HB3	1:E:371:GLU:HB3	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:37:GLN:HG3	1:F:193:LYS:HD3	1.87	0.55
1:F:210:SER:HB3	1:F:313:PRO:HD2	1.88	0.55
1:A:364:TRP:HB3	1:A:371:GLU:HB3	1.88	0.55
3:F:1001:NAG:H5	3:F:1001:NAG:H83	1.89	0.55
1:C:338:ILE:HG13	1:C:343:LEU:HD11	1.89	0.54
1:A:277:GLU:HA	1:A:280:ARG:NH1	2.22	0.54
1:E:277:GLU:HA	1:E:280:ARG:NH1	2.22	0.54
1:C:217:THR:HG22	1:C:228:ILE:HG12	1.90	0.54
1:F:338:ILE:HG13	1:F:343:LEU:HD11	1.90	0.54
1:A:2:LEU:HD12	1:A:340:GLY:HA2	1.90	0.54
1:E:2:LEU:HD12	1:E:340:GLY:HA2	1.90	0.53
1:F:61:ALA:HB2	1:F:87:PRO:HB3	1.90	0.53
1:F:337:TRP:CD1	1:F:353:PRO:HG3	2.43	0.53
1:F:76:LYS:HB2	1:A:125:LEU:HB3	1.90	0.53
1:C:189:VAL:HG13	1:C:202:ILE:HG23	1.91	0.52
1:C:210:SER:HB3	1:C:313:PRO:HD2	1.91	0.52
1:C:337:TRP:CD1	1:C:353:PRO:HG3	2.45	0.52
1:A:380:THR:HG21	1:C:401:HIS:HD2	1.74	0.52
1:A:409:LEU:HD13	1:C:326:LEU:HB2	1.92	0.52
1:E:160:THR:OG1	1:E:165:SER:O	2.23	0.51
1:F:189:VAL:HG13	1:F:202:ILE:HG23	1.92	0.51
1:F:63:LYS:HB2	1:F:63:LYS:NZ	2.25	0.51
1:C:222:TYR:HB3	1:C:235:TRP:CE2	2.46	0.51
1:A:160:THR:OG1	1:A:165:SER:O	2.24	0.51
1:A:11:LYS:HG2	1:A:363:GLN:HB2	1.93	0.50
1:E:11:LYS:HG2	1:E:363:GLN:HB2	1.94	0.50
1:E:80:HIS:HB3	1:E:109:PHE:CZ	2.46	0.50
1:E:309:ALA:HB2	1:E:375:ASN:HB3	1.94	0.50
1:E:125:LEU:HB3	1:C:76:LYS:HB2	1.94	0.50
1:F:58:LEU:HD22	1:F:165:SER:HB3	1.94	0.50
1:C:29:GLU:OE1	1:C:335:ARG:NH2	2.45	0.50
1:C:58:LEU:HD22	1:C:165:SER:HB3	1.94	0.50
1:F:217:THR:HG22	1:F:228:ILE:HG12	1.93	0.49
1:F:222:TYR:HB3	1:F:235:TRP:CE2	2.47	0.49
1:E:299:PRO:HB2	1:F:405:GLU:O	2.12	0.49
1:F:29:GLU:OE1	1:F:335:ARG:NH2	2.46	0.49
1:F:219:ARG:HH21	1:F:251:PRO:HA	1.78	0.49
1:A:173:THR:O	1:A:175:LYS:N	2.46	0.49
1:A:309:ALA:HB2	1:A:375:ASN:HB3	1.95	0.48
1:C:2:LEU:HD13	1:C:391:ILE:HD13	1.94	0.48
1:C:234:GLU:OE1	1:C:332:ARG:NH2	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:39:GLU:OE2	1:E:191:TYR:OH	2.23	0.48
1:E:173:THR:O	1:E:175:LYS:N	2.46	0.48
1:A:84:ASN:HB3	1:A:164:SER:HB3	1.96	0.48
1:E:200:GLY:HA2	1:E:215:ALA:HB2	1.95	0.48
1:F:311:LYS:HD2	1:F:389:HIS:CE1	2.49	0.48
1:C:313:PRO:HG3	1:C:335:ARG:HG2	1.95	0.47
1:F:193:LYS:HA	1:F:193:LYS:HD2	1.75	0.47
1:F:313:PRO:HG3	1:F:335:ARG:HG2	1.95	0.47
1:C:219:ARG:HH21	1:C:251:PRO:HA	1.79	0.47
1:F:2:LEU:HD13	1:F:391:ILE:HD13	1.95	0.47
1:C:193:LYS:HA	1:C:193:LYS:HD2	1.76	0.47
1:E:306:SER:CB	1:E:387:PRO:HG3	2.45	0.47
1:F:234:GLU:OE1	1:F:332:ARG:NH2	2.46	0.47
1:A:306:SER:CB	1:A:387:PRO:HG3	2.44	0.47
1:C:364:TRP:HB3	1:C:371:GLU:HB3	1.97	0.47
1:E:337:TRP:NE1	1:E:353:PRO:HG3	2.29	0.47
1:C:292:ASP:HB3	1:C:296:ARG:NH1	2.29	0.47
1:C:347:LYS:HB3	1:C:357:SER:HB3	1.96	0.47
1:F:364:TRP:HB3	1:F:371:GLU:HB3	1.97	0.47
1:C:261:GLU:OE1	1:C:263:ARG:NH2	2.48	0.46
1:F:342:VAL:HG22	1:F:385:LYS:HG2	1.97	0.46
1:F:63:LYS:HE3	1:F:85:ILE:HG21	1.98	0.46
1:F:347:LYS:HB3	1:F:357:SER:HB3	1.96	0.46
1:C:311:LYS:HD2	1:C:389:HIS:CE1	2.50	0.46
1:F:261:GLU:OE1	1:F:263:ARG:NH2	2.49	0.46
1:A:134:VAL:HB	1:A:145:ASP:HB2	1.97	0.46
1:A:200:GLY:HA2	1:A:215:ALA:HB2	1.98	0.45
1:E:123:GLU:CG	1:C:78:ILE:HB	2.46	0.45
1:F:239:ASP:OD2	1:F:241:LYS:HG2	2.15	0.45
1:E:134:VAL:HB	1:E:145:ASP:HB2	1.97	0.45
1:E:61:ALA:HB2	1:E:87:PRO:HB3	1.98	0.45
1:C:152:GLU:OE2	1:C:265:THR:HG21	2.16	0.45
1:C:342:VAL:HG22	1:C:385:LYS:HG2	1.99	0.45
1:F:78:ILE:HB	1:A:123:GLU:CG	2.47	0.45
1:F:292:ASP:HB3	1:F:296:ARG:NH1	2.32	0.45
1:F:217:THR:HG23	1:F:230:PHE:HA	1.98	0.45
1:A:337:TRP:NE1	1:A:353:PRO:HG3	2.33	0.44
1:E:26:MET:HG3	1:E:310:SER:HB2	1.99	0.44
1:A:219:ARG:HD2	1:A:250:LEU:HG	2.00	0.44
1:A:22:ARG:HG2	1:A:291:TRP:CD1	2.52	0.44
1:E:371:GLU:HB2	1:E:379:LYS:HD3	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2:LEU:HB2	1:F:338:ILE:HG22	1.99	0.44
1:C:239:ASP:OD2	1:C:241:LYS:HG2	2.16	0.44
1:E:86:LYS:HZ1	1:E:159:ASP:CG	2.20	0.44
1:E:212:MET:HG2	1:E:230:PHE:HB3	2.00	0.44
1:E:371:GLU:HB2	1:E:379:LYS:HB3	2.00	0.44
1:F:220:LEU:HD13	1:F:256:CYS:HB2	2.00	0.44
1:E:24:CYS:HA	1:E:25:PRO:HA	1.81	0.43
1:A:371:GLU:HB2	1:A:379:LYS:HD3	2.00	0.43
1:F:63:LYS:HB2	1:F:63:LYS:HZ2	1.83	0.43
1:C:43:SER:OG	1:C:44:SER:N	2.51	0.43
1:A:26:MET:HG3	1:A:310:SER:HB2	1.99	0.43
1:C:2:LEU:HB2	1:C:338:ILE:HG22	1.99	0.43
1:F:152:GLU:OE2	1:F:265:THR:HG21	2.19	0.43
1:F:43:SER:OG	1:F:44:SER:N	2.51	0.43
1:A:6:PHE:CG	1:A:7:PRO:HD2	2.53	0.43
1:C:220:LEU:HD13	1:C:256:CYS:HB2	1.99	0.43
1:E:10:THR:HB	1:E:362:THR:HG22	2.01	0.43
1:C:222:TYR:CD2	1:C:262:VAL:HG11	2.54	0.43
1:C:61:ALA:HB2	1:C:87:PRO:HB3	2.00	0.43
1:F:222:TYR:CD2	1:F:262:VAL:HG11	2.53	0.43
1:A:385:LYS:HE2	1:C:399:GLU:OE2	2.19	0.43
1:A:212:MET:HG2	1:A:230:PHE:CG	2.54	0.43
1:E:219:ARG:HD2	1:E:250:LEU:HG	2.01	0.43
1:F:337:TRP:NE1	1:F:353:PRO:HG3	2.33	0.43
1:A:378:LEU:HA	1:A:378:LEU:HD23	1.88	0.42
1:E:73:TYR:HB2	1:E:74:GLY:H	1.69	0.42
1:F:210:SER:HB3	1:F:312:SER:HB2	2.00	0.42
1:E:22:ARG:HG2	1:E:291:TRP:CD1	2.53	0.42
1:F:346:PRO:HD3	1:F:384:TYR:CE1	2.55	0.42
1:A:212:MET:HG2	1:A:230:PHE:HB3	2.00	0.42
1:A:10:THR:HB	1:A:362:THR:HG22	2.00	0.42
1:C:337:TRP:NE1	1:C:353:PRO:HG3	2.35	0.42
1:F:338:ILE:HD12	1:F:338:ILE:HA	1.88	0.42
1:F:380:THR:OG1	1:F:385:LYS:NZ	2.52	0.42
1:E:378:LEU:HD23	1:E:378:LEU:HA	1.87	0.42
1:C:217:THR:HG23	1:C:230:PHE:HA	2.01	0.42
1:F:313:PRO:CG	1:F:335:ARG:HG2	2.50	0.41
1:C:239:ASP:OD1	1:C:239:ASP:N	2.49	0.41
1:A:43:SER:OG	1:A:44:SER:N	2.52	0.41
1:C:219:ARG:NH2	1:C:251:PRO:HA	2.35	0.41
1:A:393:MET:CE	1:C:388:TRP:HB3	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:219:ARG:NH2	1:F:251:PRO:HA	2.34	0.41
1:A:371:GLU:HB2	1:A:379:LYS:HB3	2.01	0.41
1:C:42:LEU:HD12	1:C:42:LEU:HA	1.96	0.41
1:E:6:PHE:CG	1:E:7:PRO:HD2	2.55	0.41
1:F:132:HIS:CD2	1:F:147:LEU:HD22	2.55	0.41
1:C:361:TRP:NE1	1:C:363:GLN:O	2.53	0.41
1:F:254:LYS:HE2	1:F:254:LYS:HA	2.03	0.41
1:A:142:HIS:HB3	1:A:154:ASP:HB3	2.03	0.41
1:C:162:HIS:HB2	1:C:165:SER:HB2	2.02	0.41
1:E:142:HIS:HB3	1:E:154:ASP:HB3	2.02	0.41
1:E:33:GLU:HA	1:E:34:PRO:HD3	1.85	0.41
1:C:210:SER:HB3	1:C:312:SER:HB2	2.02	0.41
1:C:346:PRO:HD3	1:C:384:TYR:CE1	2.56	0.41
1:E:8:GLU:O	1:E:350:ARG:NH1	2.47	0.41
1:F:42:LEU:HD12	1:F:42:LEU:HA	1.94	0.41
1:E:212:MET:CG	1:E:230:PHE:HB3	2.51	0.41
1:E:50:THR:HA	1:E:51:PRO:HD3	1.88	0.41
1:E:299:PRO:HB2	1:F:405:GLU:C	2.41	0.41
1:E:212:MET:HG2	1:E:230:PHE:CG	2.56	0.41
1:E:65:VAL:HG22	1:E:123:GLU:HB3	2.02	0.41
1:F:162:HIS:HB2	1:F:165:SER:HB2	2.03	0.41
1:A:64:TRP:CZ3	1:A:108:GLY:HA2	2.56	0.40
1:C:338:ILE:HD12	1:C:338:ILE:HA	1.89	0.40
1:A:8:GLU:O	1:A:350:ARG:NH1	2.47	0.40
1:E:216:ARG:HB2	1:E:231:PRO:HG3	2.03	0.40
1:F:73:TYR:HB2	1:F:74:GLY:H	1.69	0.40
1:A:212:MET:CG	1:A:230:PHE:HB3	2.51	0.40
1:C:346:PRO:HD3	1:C:384:TYR:CZ	2.57	0.40
1:E:269:ASP:OD2	1:E:270:GLY:N	2.54	0.40
1:A:65:VAL:HG22	1:A:123:GLU:HB3	2.03	0.40

All (2) 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)
1:E:277:GLU:OE2	1:A:280:ARG:NH1[3_545]	2.16	0.04
1:E:280:ARG:NH1	1:A:277:GLU:OE2[3_545]	2.17	0.03

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	408/419 (97%)	397 (97%)	10 (2%)	1 (0%)	52	88
1	C	392/419 (94%)	377 (96%)	15 (4%)	0	100	100
1	E	408/419 (97%)	397 (97%)	10 (2%)	1 (0%)	52	88
1	F	392/419 (94%)	378 (96%)	14 (4%)	0	100	100
All	All	1600/1676 (96%)	1549 (97%)	49 (3%)	2 (0%)	56	90

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	174	LYS
1	A	174	LYS

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	356/364 (98%)	347 (98%)	9 (2%)	55	86
1	C	347/364 (95%)	340 (98%)	7 (2%)	63	89
1	E	356/364 (98%)	347 (98%)	9 (2%)	55	86
1	F	347/364 (95%)	341 (98%)	6 (2%)	68	91
All	All	1406/1456 (97%)	1375 (98%)	31 (2%)	60	88

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	3	SER
1	E	20	ASN
1	E	29	GLU
1	E	70	PHE
1	E	124	PHE
1	E	144	VAL
1	E	194	THR
1	E	207	LYS
1	E	342	VAL
1	F	36	LEU
1	F	70	PHE
1	F	142	HIS
1	F	254	LYS
1	F	262	VAL
1	F	273	VAL
1	A	3	SER
1	A	20	ASN
1	A	29	GLU
1	A	70	PHE
1	A	124	PHE
1	A	144	VAL
1	A	194	THR
1	A	207	LYS
1	A	342	VAL
1	C	36	LEU
1	C	70	PHE
1	C	142	HIS
1	C	210	SER
1	C	254	LYS
1	C	262	VAL
1	C	273	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	180	GLN
1	F	401	HIS
1	A	180	GLN
1	C	401	HIS

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 ⓘ

8 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$
3	NAG	A	2001	1	14,14,15	0.52	0	15,19,21	0.95	1 (6%)
3	NAG	C	2001	1	14,14,15	0.56	0	15,19,21	0.99	1 (6%)
2	SO4	E	501	-	4,4,4	0.34	0	6,6,6	0.21	0
3	NAG	F	1001	1,3	14,14,15	0.40	0	15,19,21	1.18	1 (6%)
3	NAG	F	1002	3	14,14,15	0.52	0	15,19,21	0.70	0
3	NAG	F	1003	1,3,4	14,14,15	0.58	0	15,19,21	0.97	1 (6%)
3	NAG	F	1004	3	14,14,15	0.47	0	15,19,21	0.93	0
4	FUC	F	1005	3	10,10,11	0.85	0	13,14,16	0.95	2 (15%)

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
3	NAG	A	2001	1	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	2001	1	-	0/6/23/26	0/1/1/1
2	SO4	E	501	-	-	0/0/0/0	0/0/0/0
3	NAG	F	1001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	1002	3	-	0/6/23/26	0/1/1/1
3	NAG	F	1003	1,3,4	-	0/6/23/26	0/1/1/1
3	NAG	F	1004	3	-	0/6/23/26	0/1/1/1
4	FUC	F	1005	3	-	0/0/17/20	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1005	FUC	O5-C5-C4	2.02	113.08	109.58
3	A	2001	NAG	C1-O5-C5	2.13	115.27	112.14
3	C	2001	NAG	C4-C3-C2	2.16	114.69	111.34
4	F	1005	FUC	O2-C2-C1	2.16	113.56	109.23
3	F	1003	NAG	C4-C3-C2	2.32	114.94	111.34
3	F	1001	NAG	C1-O5-C5	3.42	117.16	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1001	NAG	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	410/419 (97%)	1.09	70 (17%) 2 1	57, 105, 180, 237	0
1	C	398/419 (94%)	0.79	47 (11%) 6 2	55, 102, 165, 228	0
1	E	410/419 (97%)	1.13	79 (19%) 2 1	54, 113, 185, 245	0
1	F	398/419 (94%)	0.87	50 (12%) 5 2	56, 103, 173, 237	0
All	All	1616/1676 (96%)	0.97	246 (15%) 3 1	54, 105, 175, 245	0

All (246) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	75	PRO	12.0
1	E	75	PRO	11.2
1	A	77	TYR	9.9
1	E	116	TYR	9.7
1	E	119	VAL	9.1
1	F	72	TRP	7.2
1	A	107	LEU	6.9
1	A	108	GLY	6.9
1	A	117	ALA	6.5
1	E	64	TRP	6.4
1	C	248	HIS	6.4
1	C	393	MET	6.3
1	A	104	LEU	6.1
1	F	125	LEU	6.0
1	E	378	LEU	6.0
1	F	393	MET	5.8
1	A	116	TYR	5.7
1	A	64	TRP	5.7
1	A	71	ARG	5.6
1	E	366	LYS	5.4
1	C	115	GLY	5.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	76	LYS	5.3
1	E	76	LYS	5.3
1	A	74	GLY	5.3
1	E	124	PHE	5.2
1	A	174	LYS	5.2
1	A	114	CYS	5.0
1	E	73	TYR	5.0
1	F	124	PHE	5.0
1	F	271	ALA	4.9
1	E	107	LEU	4.9
1	A	73	TYR	4.7
1	E	113	SER	4.7
1	A	166	VAL	4.6
1	A	130	THR	4.6
1	C	114	CYS	4.6
1	C	77	TYR	4.5
1	C	71	ARG	4.5
1	E	59	CYS	4.4
1	A	321	VAL	4.4
1	F	73	TYR	4.4
1	C	116	TYR	4.4
1	C	117	ALA	4.4
1	F	71	ARG	4.4
1	C	78	ILE	4.4
1	E	172	GLN	4.3
1	E	77	TYR	4.3
1	C	76	LYS	4.3
1	A	372	ILE	4.3
1	E	65	VAL	4.3
1	C	174	LYS	4.2
1	F	402	GLU	4.1
1	F	401	HIS	4.1
1	C	72	TRP	4.1
1	F	129	ILE	4.0
1	C	271	ALA	4.0
1	F	126	VAL	4.0
1	A	78	ILE	4.0
1	E	166	VAL	3.9
1	A	115	GLY	3.9
1	A	89	ARG	3.9
1	E	384	TYR	3.9
1	F	77	TYR	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	172	GLN	3.9
1	E	62	ALA	3.9
1	E	322	ILE	3.8
1	A	100	LYS	3.8
1	C	70	PHE	3.8
1	A	16	PRO	3.8
1	E	364	TRP	3.8
1	E	343	LEU	3.7
1	E	367	TYR	3.7
1	A	124	PHE	3.7
1	E	115	GLY	3.7
1	A	165	SER	3.7
1	E	248	HIS	3.6
1	C	120	THR	3.6
1	F	117	ALA	3.6
1	C	244	ILE	3.6
1	F	119	VAL	3.6
1	A	326	LEU	3.5
1	A	128	MET	3.5
1	E	78	ILE	3.5
1	A	119	VAL	3.5
1	A	168	ILE	3.5
1	A	378	LEU	3.5
1	E	68	CYS	3.5
1	E	74	GLY	3.4
1	F	104	LEU	3.4
1	F	92	CYS	3.4
1	E	122	SER	3.4
1	E	71	ARG	3.3
1	F	63	LYS	3.3
1	F	64	TRP	3.3
1	C	68	CYS	3.2
1	F	392	GLY	3.2
1	F	248	HIS	3.2
1	E	360	ILE	3.2
1	F	62	ALA	3.2
1	A	325	THR	3.2
1	E	72	TRP	3.2
1	F	128	MET	3.2
1	E	326	LEU	3.2
1	C	121	ASP	3.2
1	E	359	ASP	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	121	ASP	3.1
1	E	58	LEU	3.1
1	E	325	THR	3.1
1	F	69	ASP	3.1
1	A	367	TYR	3.1
1	E	117	ALA	3.1
1	A	14	TRP	3.1
1	A	248	HIS	3.1
1	C	196	GLU	3.0
1	E	377	LEU	3.0
1	A	120	THR	3.0
1	F	174	LYS	2.9
1	F	127	ILE	2.9
1	E	385	LYS	2.9
1	C	177	ILE	2.9
1	E	87	PRO	2.9
1	F	103	THR	2.9
1	E	372	ILE	2.9
1	E	148	PHE	2.9
1	A	15	LYS	2.9
1	A	197	ILE	2.9
1	A	122	SER	2.8
1	E	157	TYR	2.8
1	E	161	ILE	2.8
1	F	173	THR	2.8
1	C	1	TYR	2.8
1	E	323	ASN	2.8
1	E	120	THR	2.8
1	F	120	THR	2.8
1	E	114	CYS	2.8
1	E	174	LYS	2.8
1	A	127	ILE	2.8
1	E	129	ILE	2.8
1	F	121	ASP	2.8
1	F	26	MET	2.8
1	F	246	GLU	2.8
1	F	85	ILE	2.7
1	A	322	ILE	2.7
1	A	113	SER	2.7
1	A	320	THR	2.7
1	F	101	SER	2.7
1	C	39	GLU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	104	LEU	2.6
1	C	172	GLN	2.6
1	C	69	ASP	2.6
1	E	67	THR	2.6
1	F	158	CYS	2.6
1	F	111	PRO	2.6
1	A	57	PHE	2.6
1	C	222	TYR	2.6
1	A	211	HIS	2.6
1	E	127	ILE	2.5
1	A	373	GLY	2.5
1	A	157	TYR	2.5
1	C	118	SER	2.5
1	E	15	LYS	2.5
1	E	83	HIS	2.5
1	E	89	ARG	2.4
1	F	118	SER	2.4
1	A	112	GLU	2.4
1	A	28	GLY	2.4
1	C	202	ILE	2.4
1	F	1	TYR	2.4
1	A	59	CYS	2.4
1	F	116	TYR	2.4
1	C	267	GLN	2.4
1	E	386	PHE	2.4
1	E	108	GLY	2.4
1	A	12	LEU	2.4
1	E	93	ASP	2.4
1	C	155	GLN	2.4
1	F	76	LYS	2.4
1	F	249	LEU	2.4
1	E	57	PHE	2.3
1	E	61	ALA	2.3
1	C	268	SER	2.3
1	A	368	GLY	2.3
1	C	249	LEU	2.3
1	F	60	HIS	2.3
1	A	384	TYR	2.3
1	F	148	PHE	2.3
1	E	321	VAL	2.3
1	E	16	PRO	2.3
1	E	379	LYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	276	SER	2.3
1	A	144	VAL	2.3
1	A	347	LYS	2.3
1	A	364	TRP	2.3
1	F	131	PRO	2.3
1	A	172	GLN	2.3
1	C	59	CYS	2.2
1	C	262	VAL	2.2
1	C	107	LEU	2.2
1	E	85	ILE	2.2
1	A	72	TRP	2.2
1	A	388	TRP	2.2
1	E	128	MET	2.2
1	C	119	VAL	2.2
1	E	347	LYS	2.2
1	F	244	ILE	2.2
1	C	57	PHE	2.2
1	E	383	GLY	2.2
1	E	168	ILE	2.2
1	A	129	ILE	2.2
1	A	103	THR	2.2
1	C	275	THR	2.2
1	C	73	TYR	2.1
1	A	386	PHE	2.1
1	C	220	LEU	2.1
1	E	374	PRO	2.1
1	E	373	GLY	2.1
1	F	224	GLY	2.1
1	E	363	GLN	2.1
1	A	305	LEU	2.1
1	C	250	LEU	2.1
1	A	105	VAL	2.1
1	E	123	GLU	2.1
1	F	157	TYR	2.1
1	C	246	GLU	2.1
1	C	399	GLU	2.1
1	A	11	LYS	2.1
1	C	175	LYS	2.1
1	E	109	PHE	2.1
1	A	159	ASP	2.1
1	E	361	TRP	2.1
1	A	118	SER	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	343	LEU	2.1
1	C	199	ALA	2.1
1	E	371	GLU	2.1
1	E	147	LEU	2.0
1	F	167	TRP	2.0
1	E	11	LYS	2.0
1	F	169	PRO	2.0
1	A	7	PRO	2.0
1	C	123	GLU	2.0
1	E	110	PRO	2.0
1	A	156	SER	2.0
1	F	50	THR	2.0
1	C	67	THR	2.0
1	E	365	PHE	2.0
1	A	32	LEU	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	E	501	5/5	0.98	0.30	2.08	62,69,77,80	0
3	NAG	A	2001	14/15	0.81	0.29	-	136,165,180,182	0
3	NAG	F	1002	14/15	0.75	0.71	-	202,211,216,217	0
4	FUC	F	1005	10/11	0.32	0.43	-	197,204,211,211	0
3	NAG	F	1003	14/15	0.62	0.37	-	92,173,204,212	0
3	NAG	F	1004	14/15	0.86	0.41	-	170,187,192,195	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	C	2001	14/15	0.71	0.24	-	79,167,185,189	0
3	NAG	F	1001	14/15	0.68	0.41	-	175,203,214,218	0

6.5 Other polymers [i](#)

There are no such residues in this entry.