Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:21 AM GMT

PDB ID	:	2QAD
Title	:	Structure of tyrosine-sulfated 412d antibody complexed with HIV-1 YU2 gp120 and CD4
Authors	:	Huang, C.-C.; Tang, M.; Robinson, J.; Wyatt, R.; Kwong, P.D.
Deposited on	:	2007-06-14
Resolution	:	3.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

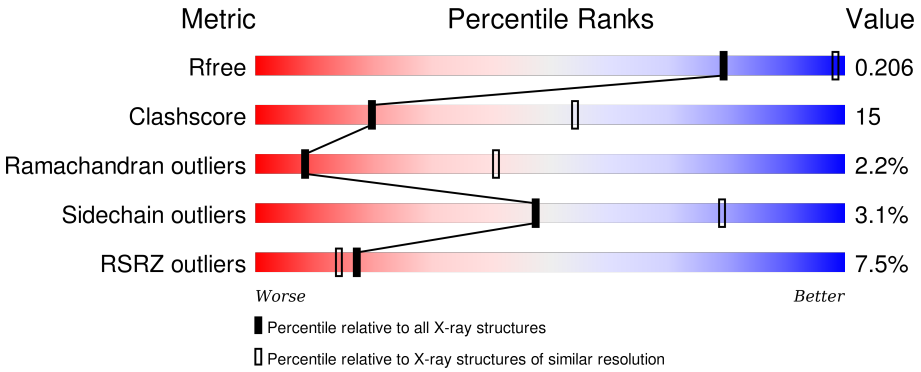
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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 <=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	322	2% 65% 33%
1	E	322	% 61% 33%
2	B	181	4% 65% 31%
2	F	181	7% 65% 32%
3	C	214	12% 64% 33%

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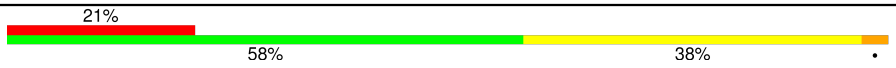
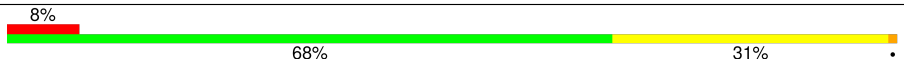
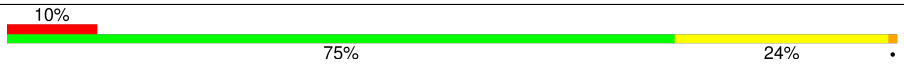
Mol	Chain	Length	Quality of chain
3	G	214	
4	D	231	
4	H	231	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	A	832	-	-	-	X
5	NAG	A	862	X	-	-	-
5	NAG	A	894	X	-	-	X
5	NAG	A	900	-	-	-	X
5	NAG	E	801	-	-	-	X
5	NAG	E	832	-	-	-	X
5	NAG	E	862	X	-	-	-
5	NAG	E	963	X	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14987 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 Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2499	1562	445	474	18			
1	E	312	Total	C	N	O	S	0	0	0
			2445	1533	430	464	18			

- Molecule 2 is a protein called T-cell surface glycoprotein CD4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	178	Total	C	N	O	S	0	0	0
			1383	865	242	272	4			
2	F	179	Total	C	N	O	S	0	0	0
			1394	874	243	273	4			

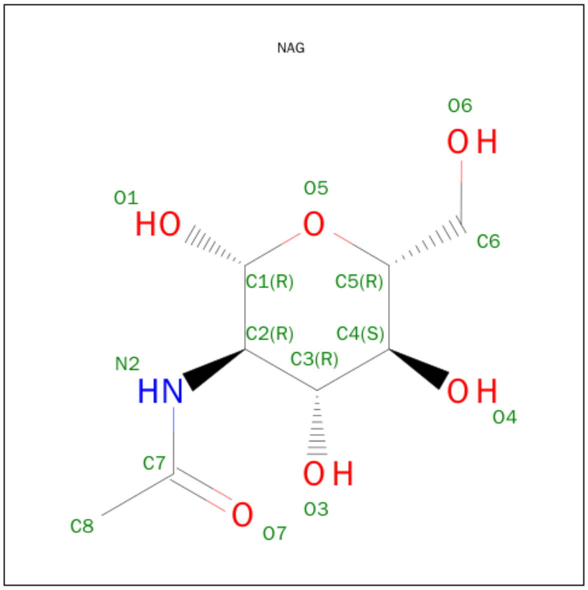
- Molecule 3 is a protein called anti-HIV-1 antibody 412d light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	213	Total	C	N	O	S	0	0	0
			1642	1024	278	334	6			
3	G	213	Total	C	N	O	S	0	0	0
			1642	1024	278	334	6			

- Molecule 4 is a protein called anti-HIV-1 antibody 412d heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	231	Total	C	N	O	S	0	0	0
			1746	1101	286	350	9			
4	H	231	Total	C	N	O	S	0	0	0
			1746	1101	286	350	9			

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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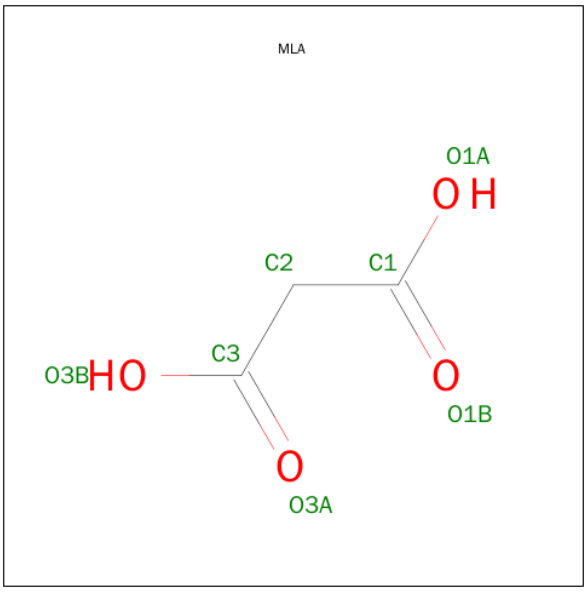
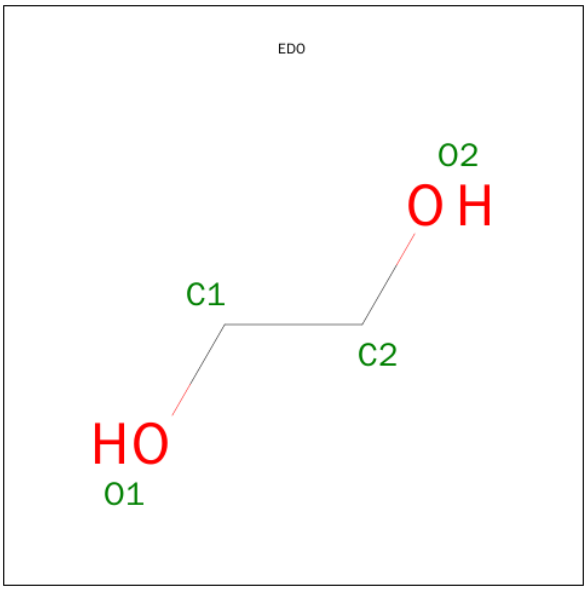
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total 14	C 8	N 1	O 5	0	0
5	A	1	Total 14	C 8	N 1	O 5	0	0
5	E	1	Total 14	C 8	N 1	O 5	0	0
5	E	1	Total 14	C 8	N 1	O 5	0	0
5	E	1	Total 14	C 8	N 1	O 5	0	0
5	E	1	Total 14	C 8	N 1	O 5	0	0
5	E	1	Total 14	C 8	N 1	O 5	0	0
5	E	1	Total 14	C 8	N 1	O 5	0	0
5	E	1	Total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

- Molecule 6 is MALONIC ACID (three-letter code: MLA) (formula: $C_3H_4O_4$).



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

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



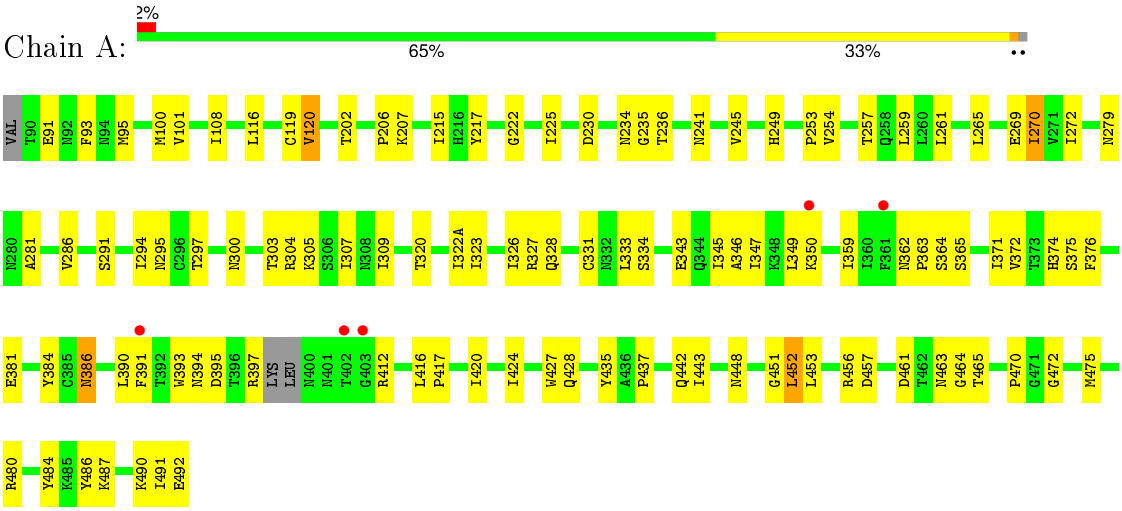
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	C	O	0	0
			4	2	2		
7	F	1	Total	C	O	0	0
			4	2	2		
7	E	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		
7	E	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		

3 Residue-property plots (i)

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

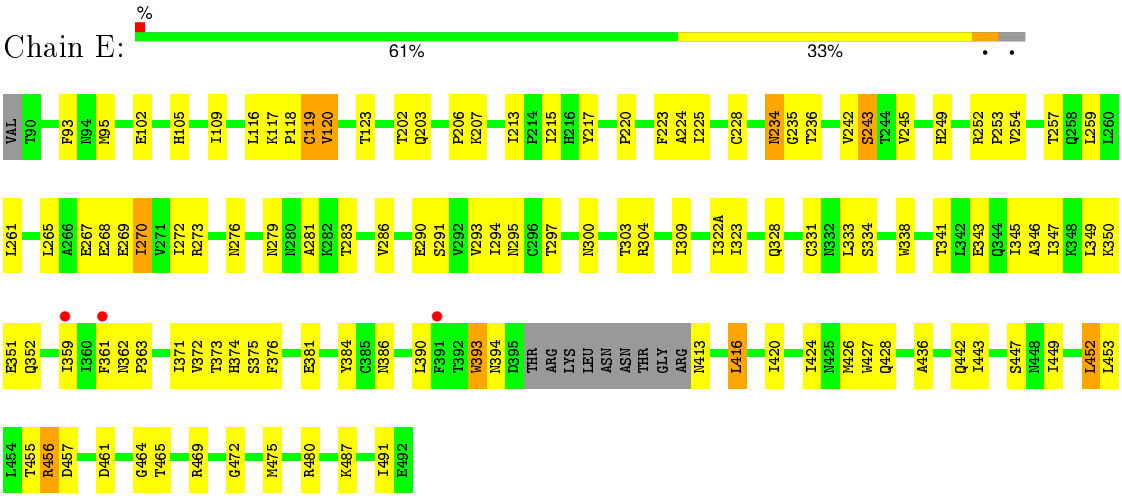
- Molecule 1: Envelope glycoprotein gp160

Chain A:



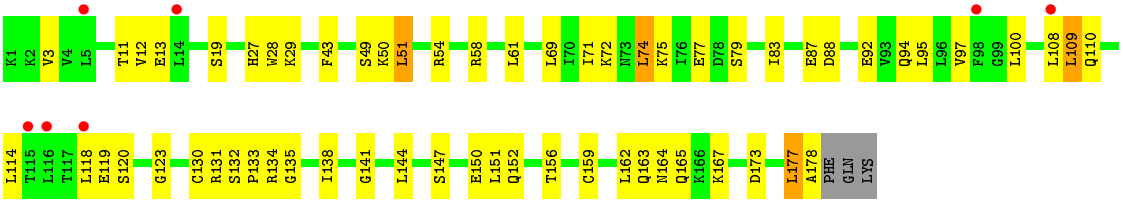
- Molecule 1: Envelope glycoprotein gp160

Chain E:



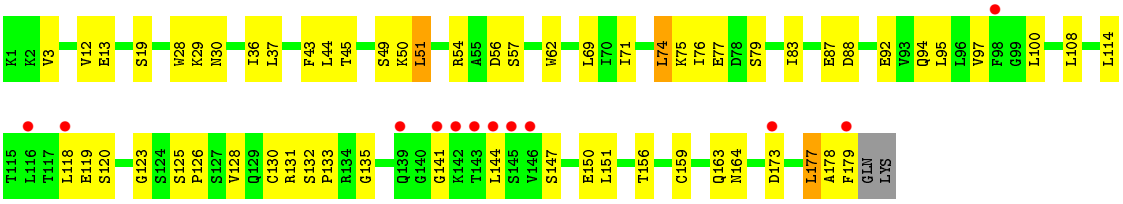
- Molecule 2: T-cell surface glycoprotein CD4

Chain B:



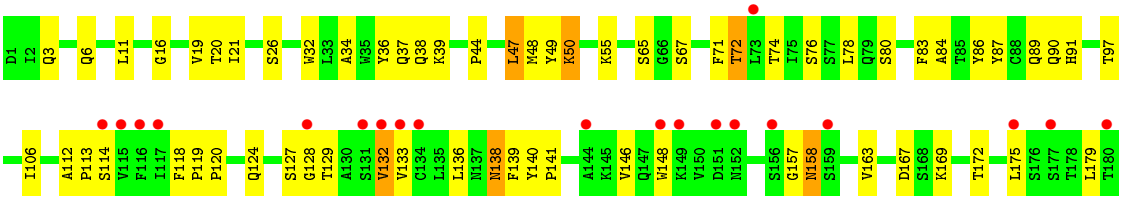
• Molecule 2: T-cell surface glycoprotein CD4

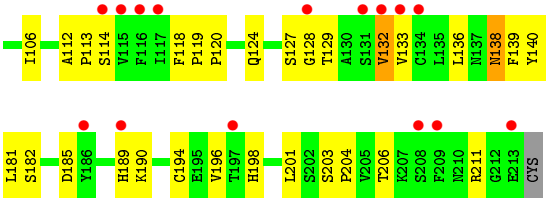
Chain F:



• Molecule 3: anti-HIV-1 antibody 412d light chain

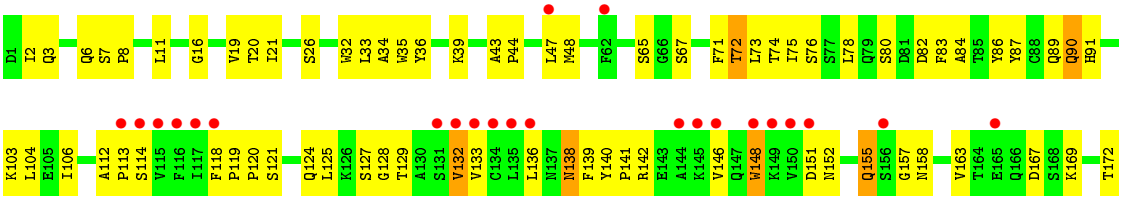
Chain C:

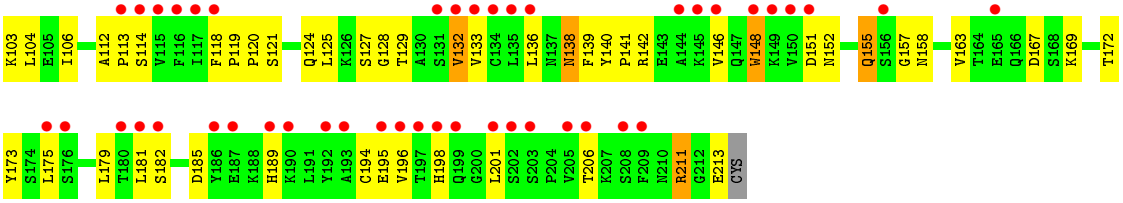




• Molecule 3: anti-HIV-1 antibody 412d light chain

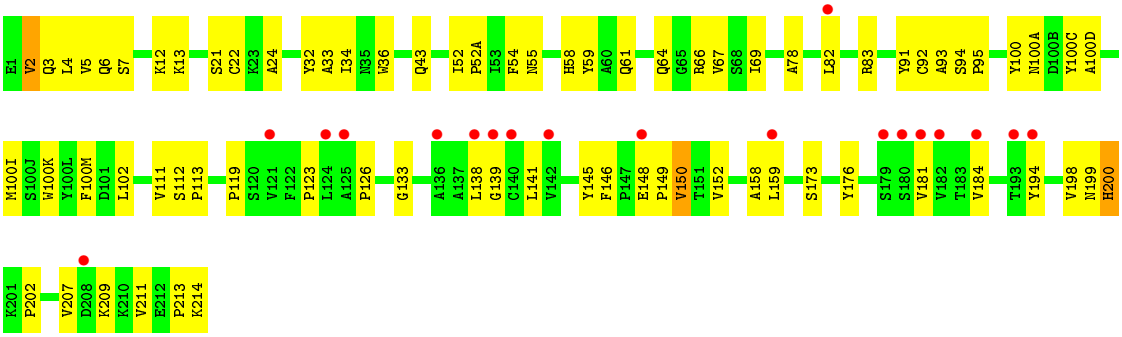
Chain G:



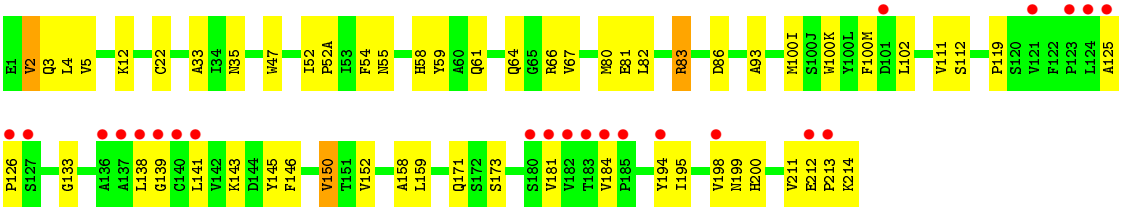


• Molecule 4: anti-HIV-1 antibody 412d heavy chain

Chain D:



- Molecule 4: anti-HIV-1 antibody 412d heavy chain



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	109.60Å 53.02Å 225.33Å 90.00° 104.64° 90.00°	Depositor
Resolution (Å)	20.00 – 3.30 49.15 – 3.31	Depositor EDS
% Data completeness (in resolution range)	66.7 (20.00-3.30) 66.4 (49.15-3.31)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 3.33Å)	Xtriage
Refinement program	CNS/PHENIX	Depositor
R, R_{free}	0.202 , 0.269 0.209 , 0.206	Depositor DCC
R_{free} test set	1268 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	93.1	Xtriage
Anisotropy	0.605	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 104.5	EDS
Estimated twinning fraction	0.034 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 25482 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	14987	wwPDB-VP
Average B, all atoms (Å^2)	157.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MLA, EDO, NAG, TYS

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	0/2546	0.47	0/3446
1	E	0.28	0/2493	0.46	0/3376
2	B	0.25	0/1402	0.44	0/1891
2	F	0.25	0/1414	0.45	0/1907
3	C	0.24	0/1677	0.41	0/2273
3	G	0.25	0/1677	0.42	0/2273
4	D	0.25	0/1757	0.43	0/2393
4	H	0.25	0/1757	0.43	0/2393
All	All	0.26	0/14723	0.44	0/19952

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

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	2499	0	2443	98	0
1	E	2445	0	2394	86	0
2	B	1383	0	1414	40	0
2	F	1394	0	1423	40	0
3	C	1642	0	1596	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1642	0	1596	66	0
4	D	1746	0	1684	53	0
4	H	1746	0	1684	41	0
5	A	224	0	208	12	0
5	E	210	0	195	6	0
6	A	7	0	3	0	0
6	B	7	0	3	0	0
6	F	7	0	3	0	0
6	H	7	0	3	0	0
7	A	4	0	6	0	0
7	C	8	0	12	0	0
7	D	4	0	6	0	0
7	E	8	0	12	1	0
7	F	4	0	6	0	0
All	All	14987	0	14691	442	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 15.

All (442) 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)
2:B:134:ARG:HH22	2:B:152:GLN:HB3	1.22	1.02
1:A:272:ILE:HG22	1:A:286:VAL:HG22	1.47	0.96
2:F:79:SER:HB3	2:F:97:VAL:HG23	1.52	0.92
4:D:126:PRO:HD2	4:D:213:PRO:HA	1.56	0.87
2:B:79:SER:HB3	2:B:97:VAL:HG23	1.57	0.86
2:B:134:ARG:NH2	2:B:152:GLN:HB3	1.89	0.86
3:C:65:SER:HB3	3:G:65:SER:HB3	1.58	0.86
1:E:224:ALA:HB2	1:E:491:ILE:HD11	1.57	0.85
1:A:397:ARG:CA	1:A:397:ARG:CG	2.54	0.85
4:H:126:PRO:HD2	4:H:213:PRO:HA	1.57	0.85
4:D:66:ARG:HH12	4:D:83:ARG:NH2	1.75	0.84
2:B:28:TRP:CD2	2:B:69:LEU:HD12	2.12	0.84
5:A:832:NAG:H62	5:A:913:NAG:H61	1.60	0.83
3:G:39:LYS:HD3	3:G:84:ALA:HB2	1.61	0.82
2:F:3:VAL:HG12	2:F:94:GLN:HB3	1.62	0.81
1:E:272:ILE:HG22	1:E:286:VAL:HG22	1.62	0.81
4:H:119:PRO:HA	4:H:145:TYR:HB3	1.64	0.79
4:H:93:ALA:HB1	4:H:100(M):PHE:HB3	1.65	0.79
4:D:93:ALA:HB1	4:D:100(M):PHE:HB3	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:119:PRO:HA	4:D:145:TYR:HB3	1.64	0.78
1:A:95:MET:HE3	1:A:235:GLY:HA3	1.66	0.77
1:E:254:VAL:HG11	1:E:261:LEU:HB2	1.66	0.77
1:E:269:GLU:HB3	5:E:789:NAG:H61	1.67	0.77
4:D:66:ARG:HH12	4:D:83:ARG:CZ	1.99	0.76
4:H:67:VAL:HG22	4:H:82:LEU:HD13	1.66	0.75
1:A:100:MET:HE1	1:A:486:TYR:HB2	1.69	0.75
1:E:343:GLU:O	1:E:347:ILE:HG12	1.88	0.74
4:H:158:ALA:HB1	4:H:194:TYR:CD1	2.22	0.74
3:G:6:GLN:HE22	3:G:87:TYR:HA	1.51	0.74
3:G:16:GLY:H	3:G:78:LEU:HB3	1.52	0.74
2:F:28:TRP:CD2	2:F:69:LEU:HD12	2.23	0.74
2:B:51:LEU:HD22	2:B:71:ILE:HD12	1.69	0.74
3:C:80:SER:HA	3:C:83:PHE:HE2	1.54	0.73
3:C:16:GLY:H	3:C:78:LEU:HB3	1.52	0.73
3:C:113:PRO:HA	3:C:139:PHE:HB3	1.70	0.72
1:A:95:MET:CE	1:A:484:TYR:HB2	2.20	0.71
1:A:309:ILE:HG22	1:E:217:TYR:HD1	1.54	0.71
3:C:190:LYS:HG3	3:C:211:ARG:HD3	1.73	0.70
3:C:90:GLN:HE21	3:C:97:THR:H	1.36	0.70
1:E:338:TRP:CE2	1:E:390:LEU:HD12	2.26	0.70
3:G:194:CYS:H	3:G:206:THR:HG21	1.57	0.70
3:G:103:LYS:HD3	3:G:142:ARG:HH12	1.57	0.69
3:G:124:GLN:HE22	4:H:141:LEU:HD23	1.57	0.69
4:H:66:ARG:CZ	4:H:83:ARG:NH1	2.56	0.69
2:B:3:VAL:HG12	2:B:94:GLN:HB3	1.75	0.69
3:C:194:CYS:H	3:C:206:THR:HG21	1.58	0.68
1:A:93:PHE:HE1	1:A:487:LYS:HB3	1.58	0.68
2:B:28:TRP:CG	2:B:69:LEU:HD12	2.29	0.68
3:C:141:PRO:HD2	3:C:198:HIS:NE2	2.08	0.67
3:G:146:VAL:HG13	3:G:196:VAL:HG22	1.75	0.67
1:A:270:ILE:H	1:A:270:ILE:HD12	1.58	0.67
1:A:303:THR:HG23	4:D:100(C):TYS:HE2	1.77	0.67
1:A:254:VAL:HG11	1:A:261:LEU:HB2	1.77	0.67
3:G:113:PRO:HA	3:G:139:PHE:HB3	1.76	0.67
1:A:215:ILE:HD12	1:A:253:PRO:HG3	1.77	0.67
1:A:222:GLY:O	1:A:491:ILE:HG22	1.95	0.66
1:A:225:ILE:HB	1:A:245:VAL:HG23	1.77	0.66
1:A:303:THR:HG22	1:A:322(A):ILE:HG12	1.77	0.66
4:D:139:GLY:HA3	4:D:181:VAL:HG12	1.78	0.66
3:G:112:ALA:HB1	3:G:201:LEU:HD11	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:39:LYS:HD3	3:C:84:ALA:HB2	1.77	0.66
1:A:309:ILE:O	1:E:217:TYR:HA	1.95	0.65
1:E:303:THR:HG22	1:E:322(A):ILE:HG12	1.77	0.65
3:G:132:VAL:HG21	3:G:148:TRP:HH2	1.62	0.65
1:A:120:VAL:HB	1:A:202:THR:HG22	1.77	0.65
3:G:148:TRP:HE3	3:G:155:GLN:HG3	1.60	0.65
1:A:279:ASN:HA	5:A:776:NAG:H61	1.77	0.64
3:G:136:LEU:HD13	3:G:175:LEU:HD11	1.80	0.64
1:A:350:LYS:HE3	1:A:359:ILE:HG13	1.80	0.63
2:B:75:LYS:O	2:B:97:VAL:HG11	1.99	0.63
1:A:362:ASN:OD1	1:A:363:PRO:HD2	1.99	0.63
3:C:179:LEU:HD21	3:C:181:LEU:HD12	1.81	0.63
3:C:11:LEU:HD21	3:C:19:VAL:HG11	1.80	0.62
3:C:163:VAL:HG12	3:C:175:LEU:HB3	1.81	0.62
3:G:65:SER:HB2	3:G:72:THR:HG23	1.80	0.62
1:A:95:MET:HE1	1:A:484:TYR:HB2	1.82	0.62
1:A:456:ARG:HG2	1:A:457:ASP:N	2.15	0.62
1:E:120:VAL:HB	1:E:202:THR:HG22	1.81	0.62
3:C:80:SER:HA	3:C:83:PHE:CE2	2.36	0.61
1:A:397:ARG:NH2	5:A:894:NAG:H61	2.16	0.61
3:G:163:VAL:HG12	3:G:175:LEU:HB3	1.82	0.61
4:H:3:GLN:HG2	4:H:4:LEU:H	1.66	0.60
3:C:158:ASN:HB2	3:C:179:LEU:HD12	1.82	0.60
1:E:456:ARG:HG3	1:E:457:ASP:N	2.16	0.60
3:G:132:VAL:HG21	3:G:148:TRP:CH2	2.36	0.60
4:D:158:ALA:HB1	4:D:194:TYR:CD1	2.37	0.60
1:A:95:MET:HE2	1:A:484:TYR:HB2	1.84	0.60
3:G:124:GLN:NE2	4:H:141:LEU:HD23	2.17	0.60
4:D:150:VAL:HG23	4:D:199:ASN:O	2.02	0.59
2:B:50:LYS:HE2	2:B:77:GLU:HG3	1.84	0.59
3:C:6:GLN:HE22	3:C:87:TYR:HA	1.67	0.59
2:F:83:ILE:HG12	2:F:92:GLU:HG2	1.83	0.59
4:D:7:SER:HB2	4:D:21:SER:OG	2.02	0.59
3:C:65:SER:HB2	3:C:72:THR:HG23	1.84	0.59
1:E:283:THR:HG22	1:E:455:THR:HG22	1.83	0.59
1:A:364:SER:O	5:A:862:NAG:H81	2.03	0.59
4:D:13:LYS:HD2	4:D:13:LYS:H	1.68	0.59
2:B:165:GLN:HG2	2:B:165:GLN:O	2.02	0.59
2:B:150:GLU:HG2	2:B:151:LEU:H	1.68	0.59
4:D:67:VAL:HG22	4:D:82:LEU:HD13	1.85	0.58
4:H:138:LEU:HD22	4:H:211:VAL:HG11	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:384:TYR:OH	1:E:424:ILE:HG22	2.03	0.58
4:D:3:GLN:HG2	4:D:4:LEU:H	1.67	0.58
1:E:350:LYS:HE3	1:E:359:ILE:HG13	1.84	0.58
4:D:52:ILE:HG21	4:D:54:PHE:HD2	1.69	0.58
3:C:90:GLN:NE2	3:C:97:THR:H	2.00	0.58
4:H:66:ARG:CZ	4:H:83:ARG:HH11	2.15	0.58
1:E:276:ASN:ND2	1:E:279:ASN:HB2	2.18	0.58
1:E:207:LYS:HE3	1:E:436:ALA:HB3	1.86	0.58
4:D:12:LYS:O	4:D:111:VAL:HA	2.04	0.58
3:C:140:TYR:CG	3:C:141:PRO:HA	2.38	0.58
2:F:54:ARG:NH1	2:F:74:LEU:HA	2.19	0.58
4:H:12:LYS:O	4:H:111:VAL:HA	2.04	0.58
1:E:381:GLU:HB3	1:E:420:ILE:HD13	1.85	0.57
2:B:156:THR:HG22	2:B:173:ASP:OD1	2.04	0.57
1:A:265:LEU:HD21	1:A:291:SER:HB3	1.84	0.57
3:G:20:THR:HG22	3:G:74:THR:HG23	1.86	0.57
1:A:397:ARG:HH22	5:A:894:NAG:H61	1.69	0.57
4:D:159:LEU:HD22	4:D:184:VAL:HG12	1.86	0.57
4:H:52:ILE:HG21	4:H:54:PHE:HD2	1.69	0.57
4:D:152:VAL:HG13	4:D:198:VAL:HG22	1.86	0.57
4:H:150:VAL:HG23	4:H:199:ASN:O	2.04	0.57
3:C:89:GLN:HG2	3:C:90:GLN:N	2.21	0.56
3:C:118:PHE:HB2	3:C:133:VAL:HB	1.87	0.56
3:G:179:LEU:HD21	3:G:181:LEU:HD12	1.87	0.56
3:C:136:LEU:HD13	3:C:175:LEU:HD11	1.88	0.56
2:B:54:ARG:NH1	2:B:74:LEU:HA	2.21	0.56
4:D:66:ARG:NH1	4:D:83:ARG:CZ	2.67	0.56
2:F:50:LYS:HE2	2:F:77:GLU:HG3	1.86	0.56
1:A:217:TYR:HD1	1:E:309:ILE:HG22	1.71	0.56
3:G:148:TRP:CH2	3:G:179:LEU:HB2	2.41	0.56
2:F:118:LEU:HD21	2:F:120:SER:HB3	1.88	0.56
2:F:51:LEU:HD22	2:F:71:ILE:HD12	1.87	0.55
2:B:130:CYS:HA	2:B:159:CYS:HA	1.89	0.55
1:A:381:GLU:HB3	1:A:420:ILE:HD13	1.89	0.55
1:A:343:GLU:O	1:A:347:ILE:HG12	2.05	0.55
1:A:456:ARG:HG2	1:A:457:ASP:H	1.72	0.55
3:G:83:PHE:CE1	3:G:106:ILE:HG12	2.42	0.55
3:G:195:GLU:HG3	3:G:206:THR:OG1	2.07	0.55
4:D:145:TYR:CE2	4:D:150:VAL:HG11	2.42	0.55
3:G:114:SER:O	3:G:136:LEU:HA	2.07	0.55
4:H:52:ILE:HB	4:H:54:PHE:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:265:LEU:HD21	1:E:291:SER:HB3	1.89	0.55
3:G:140:TYR:CG	3:G:141:PRO:HA	2.42	0.55
3:C:114:SER:O	3:C:136:LEU:HA	2.07	0.54
4:H:33:ALA:HB2	4:H:52(A):PRO:HG3	1.90	0.54
1:A:346:ALA:HB1	1:A:359:ILE:HG12	1.89	0.54
3:C:194:CYS:H	3:C:206:THR:CG2	2.21	0.54
1:E:346:ALA:HB1	1:E:359:ILE:HG12	1.88	0.54
3:G:11:LEU:HD21	3:G:19:VAL:HG11	1.89	0.54
4:H:143:LYS:HE2	4:H:171:GLN:HE21	1.73	0.54
3:C:91:HIS:HB2	4:D:100(K):TRP:HB2	1.89	0.54
2:B:83:ILE:HG12	2:B:92:GLU:HG2	1.89	0.54
3:C:185:ASP:O	3:C:189:HIS:HD2	1.90	0.54
1:E:361:PHE:HD2	1:E:393:TRP:HD1	1.56	0.54
3:G:158:ASN:HB2	3:G:179:LEU:HD12	1.90	0.54
4:D:52:ILE:HB	4:D:54:PHE:HB2	1.89	0.53
4:D:138:LEU:HD22	4:D:211:VAL:HG11	1.90	0.53
1:E:93:PHE:HE2	1:E:228:CYS:HB2	1.72	0.53
4:D:33:ALA:HB2	4:D:52(A):PRO:HG3	1.90	0.53
4:D:54:PHE:O	4:D:55:ASN:HB3	2.09	0.53
1:E:427:TRP:CE3	1:E:475:MET:HG3	2.43	0.53
3:G:189:HIS:O	3:G:211:ARG:HD2	2.07	0.53
4:H:184:VAL:HG11	4:H:194:TYR:HE2	1.74	0.53
1:E:93:PHE:CE2	1:E:228:CYS:HB2	2.44	0.53
3:G:118:PHE:HB2	3:G:133:VAL:HB	1.91	0.53
1:A:397:ARG:HH12	5:A:894:NAG:H4	1.73	0.53
1:A:453:LEU:HD13	1:A:472:GLY:HA2	1.91	0.53
3:C:3:GLN:H	3:C:26:SER:HB2	1.73	0.53
1:E:93:PHE:HE1	1:E:487:LYS:HB3	1.72	0.53
3:G:194:CYS:H	3:G:206:THR:CG2	2.20	0.53
3:C:20:THR:HG22	3:C:74:THR:HG23	1.89	0.53
1:E:452:LEU:HD23	1:E:452:LEU:N	2.24	0.53
2:B:132:SER:HB2	2:B:133:PRO:HD2	1.91	0.52
1:E:362:ASN:HD22	1:E:469:ARG:HH12	1.57	0.52
3:G:136:LEU:HB2	3:G:175:LEU:HG	1.91	0.52
4:H:54:PHE:O	4:H:55:ASN:HB3	2.09	0.52
3:G:91:HIS:HB2	4:H:100(K):TRP:HB2	1.91	0.52
1:A:95:MET:HE3	1:A:235:GLY:CA	2.37	0.52
1:A:393:TRP:CZ2	1:A:395:ASP:HA	2.44	0.52
4:H:3:GLN:HG2	4:H:4:LEU:N	2.25	0.51
2:B:138:ILE:HG22	2:B:144:LEU:HD11	1.92	0.51
2:B:134:ARG:NH2	2:B:152:GLN:O	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:MET:HG2	1:A:235:GLY:O	2.10	0.51
3:C:158:ASN:O	3:C:179:LEU:HD12	2.09	0.51
2:B:162:LEU:HG	2:B:167:LYS:HB3	1.91	0.51
1:E:345:ILE:O	1:E:349:LEU:HG	2.11	0.51
2:B:28:TRP:HA	2:B:83:ILE:O	2.11	0.51
2:F:156:THR:HG22	2:F:173:ASP:OD1	2.11	0.51
3:G:80:SER:HA	3:G:83:PHE:HE2	1.76	0.51
3:G:141:PRO:HD2	3:G:198:HIS:NE2	2.25	0.51
4:H:35:ASN:HB3	4:H:47:TRP:HE1	1.76	0.50
1:A:294:ILE:HG13	1:A:333:LEU:HG	1.91	0.50
2:F:132:SER:HB2	2:F:133:PRO:HD2	1.92	0.50
1:E:453:LEU:HD13	1:E:472:GLY:HA2	1.92	0.50
4:D:123:PRO:HG3	4:D:209:LYS:HE3	1.93	0.50
2:F:75:LYS:O	2:F:97:VAL:HG11	2.12	0.50
2:F:130:CYS:HA	2:F:159:CYS:HA	1.93	0.50
4:D:43:GLN:OE1	4:D:43:GLN:HA	2.12	0.50
1:E:270:ILE:H	1:E:270:ILE:HD12	1.77	0.50
2:B:177:LEU:HD13	2:B:178:ALA:N	2.26	0.50
2:F:56:ASP:CG	2:F:57:SER:H	2.15	0.50
3:G:89:GLN:HG2	3:G:90:GLN:N	2.27	0.50
1:A:427:TRP:CE3	1:A:475:MET:HG3	2.47	0.50
1:A:100:MET:HE1	1:A:486:TYR:CB	2.40	0.50
2:F:28:TRP:HA	2:F:83:ILE:O	2.12	0.50
1:E:102:GLU:OE1	1:E:102:GLU:HA	2.12	0.50
1:A:281:ALA:HB2	2:B:29:LYS:NZ	2.27	0.50
4:D:93:ALA:HA	4:D:102:LEU:O	2.12	0.49
1:E:95:MET:O	1:E:480:ARG:HD3	2.12	0.49
4:H:93:ALA:HA	4:H:102:LEU:O	2.11	0.49
4:D:3:GLN:HG2	4:D:4:LEU:N	2.27	0.49
4:D:6:GLN:NE2	4:D:92:CYS:N	2.60	0.49
1:A:91:GLU:OE1	1:A:91:GLU:HA	2.11	0.49
1:E:105:HIS:NE2	1:E:109:ILE:HD11	2.28	0.49
3:C:34:ALA:HA	3:C:48:MET:O	2.13	0.49
2:B:118:LEU:HD21	2:B:120:SER:HB3	1.94	0.49
1:E:491:ILE:HA	7:E:7:EDO:H21	1.94	0.49
2:F:12:VAL:HG22	2:F:13:GLU:N	2.28	0.49
1:E:95:MET:HE1	1:E:273:ARG:HD3	1.94	0.49
3:C:138:ASN:HA	3:C:172:THR:HB	1.95	0.49
2:B:49:SER:HB2	2:B:51:LEU:HD12	1.95	0.48
1:E:371:ILE:HD13	2:F:45:THR:HG22	1.96	0.48
3:G:34:ALA:HA	3:G:48:MET:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:THR:HG23	5:A:734:NAG:H62	1.95	0.48
3:C:112:ALA:HB1	3:C:201:LEU:HD11	1.94	0.48
2:B:109:LEU:HD23	2:B:110:GLN:H	1.78	0.48
2:F:75:LYS:HD2	2:F:75:LYS:N	2.29	0.48
1:A:93:PHE:CE1	1:A:487:LYS:HB3	2.45	0.48
3:G:138:ASN:HA	3:G:172:THR:HB	1.95	0.48
1:E:225:ILE:HB	1:E:245:VAL:CG2	2.43	0.48
3:C:50:LYS:HE2	3:C:50:LYS:HB3	1.55	0.48
3:G:21:ILE:HD12	3:G:73:LEU:HD23	1.96	0.48
4:H:145:TYR:CE2	4:H:150:VAL:HG11	2.48	0.48
2:F:28:TRP:CG	2:F:69:LEU:HD12	2.48	0.48
1:A:230:ASP:OD1	1:A:241:ASN:HB2	2.14	0.48
2:F:57:SER:HG	2:F:62:TRP:HE1	1.60	0.48
1:A:309:ILE:HD12	1:E:215:ILE:HD12	1.95	0.48
3:G:181:LEU:HD22	3:G:185:ASP:OD2	2.14	0.48
1:E:333:LEU:HD21	1:E:449:ILE:HD11	1.95	0.48
1:A:119:CYS:HB3	4:D:100(I):MET:HG3	1.96	0.48
1:E:269:GLU:CB	5:E:789:NAG:H61	2.40	0.48
1:E:347:ILE:HG22	1:E:351:GLU:OE2	2.14	0.47
3:G:121:SER:O	3:G:125:LEU:HG	2.14	0.47
2:B:87:GLU:O	2:B:88:ASP:HB2	2.14	0.47
4:H:139:GLY:HA3	4:H:181:VAL:HG12	1.96	0.47
1:E:293:VAL:O	1:E:333:LEU:HD23	2.14	0.47
1:E:375:SER:O	1:E:376:PHE:HB3	2.14	0.47
4:D:52:ILE:HD11	4:D:58:HIS:CD2	2.50	0.47
4:H:159:LEU:HD22	4:H:184:VAL:HG12	1.96	0.47
4:H:52:ILE:HD11	4:H:58:HIS:CD2	2.49	0.47
1:E:206:PRO:HG3	3:G:32:TRP:HZ2	1.79	0.47
3:G:142:ARG:HB2	3:G:173:TYR:CE2	2.49	0.47
2:F:76:ILE:HD12	2:F:119:GLU:HG2	1.97	0.47
1:A:269:GLU:HB3	5:A:789:NAG:H61	1.96	0.47
3:C:167:ASP:OD2	3:C:169:LYS:HB2	2.15	0.47
1:A:463:ASN:OD1	5:A:963:NAG:O5	2.31	0.47
1:A:225:ILE:HB	1:A:245:VAL:CG2	2.42	0.47
3:C:146:VAL:HG22	3:C:196:VAL:HG13	1.96	0.47
1:A:333:LEU:HD13	1:A:390:LEU:HD11	1.97	0.47
3:G:136:LEU:HD22	3:G:175:LEU:HD21	1.96	0.46
1:A:297:THR:HA	1:A:443:ILE:O	2.15	0.46
1:E:242:VAL:HG22	1:E:243:SER:N	2.29	0.46
1:A:279:ASN:HB2	5:A:776:NAG:O5	2.15	0.46
1:E:119:CYS:HB3	4:H:100(I):MET:HG3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:124:GLN:HE22	4:D:141:LEU:HD23	1.80	0.46
2:F:131:ARG:HG3	2:F:135:GLY:HA2	1.97	0.46
1:E:381:GLU:HG3	1:E:443:ILE:CD1	2.45	0.46
3:C:146:VAL:HG13	3:C:196:VAL:HG22	1.96	0.46
1:A:215:ILE:HG21	1:E:309:ILE:HD12	1.97	0.46
1:A:291:SER:HB2	1:A:448:ASN:HB3	1.97	0.46
2:F:49:SER:HB2	2:F:51:LEU:HD12	1.98	0.46
4:H:5:VAL:O	4:H:22:CYS:HA	2.15	0.46
3:G:3:GLN:H	3:G:26:SER:HB2	1.80	0.46
3:G:148:TRP:O	3:G:155:GLN:HB2	2.16	0.46
3:G:129:THR:HA	3:G:182:SER:HA	1.98	0.46
3:G:2:ILE:HD12	3:G:90:GLN:NE2	2.32	0.45
1:E:371:ILE:HD11	2:F:43:PHE:HB2	1.98	0.45
4:D:34:ILE:HD12	4:D:78:ALA:HB2	1.98	0.45
4:D:5:VAL:O	4:D:22:CYS:HA	2.16	0.45
1:A:384:TYR:OH	1:A:424:ILE:HG22	2.16	0.45
1:A:303:THR:CG2	4:D:100(C):TYS:HE2	2.44	0.45
1:E:119:CYS:HA	1:E:203:GLN:O	2.16	0.45
3:G:167:ASP:OD2	3:G:169:LYS:HB2	2.16	0.45
1:A:215:ILE:HD13	1:E:309:ILE:CD1	2.47	0.45
3:G:119:PRO:HA	3:G:120:PRO:HD2	1.84	0.45
1:A:345:ILE:O	1:A:349:LEU:HG	2.16	0.45
4:D:214:LYS:OXT	4:D:214:LYS:HG2	2.17	0.45
1:E:413:ASN:HB2	5:E:913:NAG:C7	2.46	0.45
2:F:54:ARG:HH12	2:F:74:LEU:HA	1.81	0.45
3:C:129:THR:HA	3:C:182:SER:HA	1.99	0.45
3:G:75:ILE:HD12	3:G:75:ILE:N	2.31	0.45
1:A:327:ARG:HD2	4:D:100:TYS:OH	2.16	0.45
3:G:21:ILE:O	3:G:72:THR:HA	2.17	0.45
3:G:118:PHE:HA	3:G:119:PRO:HD2	1.80	0.45
3:C:37:GLN:N	3:C:47:LEU:HD21	2.32	0.45
1:E:381:GLU:HG3	1:E:443:ILE:HD13	1.98	0.45
4:H:152:VAL:HG13	4:H:198:VAL:HG22	1.99	0.45
3:C:21:ILE:O	3:C:72:THR:HA	2.17	0.44
3:G:155:GLN:HA	3:G:155:GLN:OE1	2.17	0.44
1:A:442:GLN:HG2	1:A:443:ILE:N	2.32	0.44
4:H:61:GLN:HA	4:H:64:GLN:HG2	1.99	0.44
1:A:326:ILE:HG23	4:D:100(A):ASN:OD1	2.16	0.44
1:E:254:VAL:HG13	5:E:762:NAG:H83	1.98	0.44
3:C:67:SER:HA	3:C:71:PHE:CE1	2.52	0.44
1:A:295:ASN:O	1:A:331:CYS:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ILE:HD13	1:A:253:PRO:HB3	2.00	0.44
1:A:350:LYS:HE3	1:A:359:ILE:CG1	2.47	0.44
2:F:37:LEU:HD11	2:F:44:LEU:HD11	2.00	0.44
1:E:220:PRO:HG2	1:E:223:PHE:CD2	2.52	0.44
2:F:150:GLU:HG2	2:F:151:LEU:H	1.82	0.44
2:F:177:LEU:HD11	2:F:179:PHE:CE1	2.52	0.44
1:E:290:GLU:HB2	5:E:789:NAG:O7	2.17	0.44
4:D:6:GLN:NE2	4:D:92:CYS:H	2.15	0.44
2:F:30:ASN:HB3	2:F:36:ILE:HD11	1.99	0.44
1:E:372:VAL:HG23	1:E:373:THR:HG23	1.99	0.44
2:F:79:SER:HB2	2:F:95:LEU:O	2.18	0.44
1:E:347:ILE:O	1:E:351:GLU:HG3	2.18	0.44
1:E:371:ILE:HD11	2:F:43:PHE:CB	2.47	0.44
4:D:24:ALA:HB1	4:D:32:TYR:CZ	2.53	0.44
3:G:151:ASP:O	3:G:152:ASN:HB2	2.18	0.44
3:C:124:GLN:NE2	4:D:141:LEU:HD23	2.33	0.44
1:E:252:ARG:HA	1:E:253:PRO:HD2	1.77	0.44
4:H:83:ARG:NH2	4:H:86:ASP:OD2	2.51	0.43
1:A:119:CYS:SG	1:A:435:TYR:HA	2.57	0.43
1:A:412:ARG:HD3	1:A:412:ARG:HA	1.74	0.43
2:B:134:ARG:HE	2:B:134:ARG:HB2	1.51	0.43
1:E:390:LEU:HD13	1:E:390:LEU:HA	1.87	0.43
1:A:206:PRO:HG3	3:C:32:TRP:CZ2	2.53	0.43
4:H:2:VAL:O	4:H:2:VAL:HG22	2.17	0.43
1:A:427:TRP:CE2	1:A:428:GLN:HG3	2.54	0.43
2:B:12:VAL:HG22	2:B:13:GLU:N	2.34	0.43
2:B:119:GLU:OE1	2:B:119:GLU:HA	2.18	0.43
1:A:416:LEU:HD23	1:A:416:LEU:H	1.83	0.43
4:H:66:ARG:NE	4:H:83:ARG:NH1	2.66	0.43
3:G:33:LEU:HG	3:G:34:ALA:N	2.33	0.43
4:D:61:GLN:HA	4:D:64:GLN:HG2	2.01	0.43
2:F:108:LEU:HD11	2:F:114:LEU:HD23	1.99	0.43
2:F:144:LEU:HD23	2:F:144:LEU:HA	1.85	0.43
4:H:212:GLU:HA	4:H:213:PRO:HD2	1.84	0.43
1:E:442:GLN:HG2	1:E:443:ILE:N	2.33	0.43
1:A:397:ARG:NH1	5:A:894:NAG:H4	2.34	0.43
1:A:452:LEU:N	1:A:452:LEU:HD23	2.33	0.43
1:E:341:THR:O	1:E:345:ILE:HG13	2.18	0.43
3:C:158:ASN:HB2	3:C:179:LEU:CD1	2.48	0.43
1:E:206:PRO:HG3	3:G:32:TRP:CZ2	2.53	0.43
1:A:206:PRO:HG3	3:C:32:TRP:HZ2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:58:ARG:HB2	2:B:61:LEU:HD12	2.00	0.43
1:A:451:GLY:C	1:A:452:LEU:HD23	2.39	0.43
2:F:87:GLU:O	2:F:88:ASP:HB2	2.18	0.43
2:B:79:SER:HB2	2:B:95:LEU:O	2.18	0.43
1:E:265:LEU:N	1:E:265:LEU:HD12	2.33	0.43
1:E:93:PHE:CE1	1:E:487:LYS:HB3	2.52	0.43
1:A:394:ASN:O	1:A:395:ASP:HB3	2.19	0.43
4:D:6:GLN:HE22	4:D:91:TYR:HA	1.82	0.43
3:C:119:PRO:HA	3:C:120:PRO:HD2	1.83	0.43
1:A:101:VAL:HG21	1:A:480:ARG:HG2	2.00	0.43
4:H:214:LYS:HG2	4:H:214:LYS:OXT	2.18	0.43
3:G:33:LEU:HG	3:G:34:ALA:H	1.84	0.43
3:G:7:SER:HA	3:G:8:PRO:HA	1.82	0.43
1:E:297:THR:HA	1:E:443:ILE:O	2.19	0.42
4:H:112:SER:HB3	4:H:146:PHE:CZ	2.54	0.42
1:A:391:PHE:CD2	1:A:470:PRO:HG3	2.54	0.42
1:A:108:ILE:CD1	1:A:253:PRO:HB3	2.49	0.42
3:G:36:TYR:O	3:G:86:TYR:HA	2.19	0.42
3:C:49:TYR:CE1	3:C:55:LYS:HD2	2.55	0.42
2:B:138:ILE:O	2:B:144:LEU:HD21	2.20	0.42
1:E:304:ARG:HG3	1:E:323:ILE:HD13	2.01	0.42
1:A:207:LYS:HD3	1:A:207:LYS:HA	1.79	0.42
2:B:132:SER:HB2	2:B:133:PRO:CD	2.49	0.42
1:E:294:ILE:HG13	1:E:333:LEU:HG	2.02	0.42
1:E:234:ASN:HB3	1:E:236:THR:O	2.20	0.42
3:G:80:SER:HA	3:G:83:PHE:CE2	2.54	0.42
3:C:36:TYR:O	3:C:86:TYR:HA	2.19	0.42
1:A:437:PRO:O	4:D:100(D):ALA:HB2	2.19	0.42
2:B:11:THR:HG22	2:B:72:LYS:HB3	2.01	0.42
4:D:112:SER:HA	4:D:113:PRO:HD3	1.90	0.42
2:F:163:GLN:HG3	2:F:164:ASN:OD1	2.19	0.42
2:B:108:LEU:HD11	2:B:114:LEU:HD23	2.02	0.42
4:H:81:GLU:HG2	4:H:82:LEU:N	2.35	0.42
4:D:184:VAL:HG11	4:D:194:TYR:HE2	1.85	0.42
1:A:381:GLU:HG3	1:A:443:ILE:CD1	2.50	0.42
1:A:381:GLU:HG3	1:A:443:ILE:HD13	2.02	0.42
2:B:163:GLN:O	2:B:164:ASN:HB2	2.20	0.42
3:C:132:VAL:HB	3:C:148:TRP:HH2	1.84	0.42
3:G:67:SER:HA	3:G:71:PHE:CE1	2.55	0.42
3:G:35:TRP:CD1	3:G:73:LEU:HD13	2.55	0.41
3:G:158:ASN:O	3:G:179:LEU:HD12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:LEU:HA	1:A:417:PRO:HD3	1.77	0.41
1:E:267:GLU:HG3	1:E:268:GLU:HG3	2.01	0.41
1:E:272:ILE:HD13	1:E:349:LEU:HD23	2.02	0.41
1:A:416:LEU:HD23	1:A:416:LEU:N	2.34	0.41
4:D:112:SER:HB3	4:D:146:PHE:CZ	2.55	0.41
3:C:38:GLN:NE2	3:C:44:PRO:HG3	2.35	0.41
4:D:2:VAL:HG13	4:D:2:VAL:O	2.20	0.41
1:A:309:ILE:HG22	1:E:217:TYR:CD1	2.44	0.41
2:F:100:LEU:HD21	2:F:118:LEU:HB2	2.02	0.41
1:A:257:THR:O	1:A:259:LEU:N	2.48	0.41
1:E:257:THR:C	1:E:259:LEU:H	2.22	0.41
1:E:234:ASN:HA	1:E:234:ASN:HD22	1.66	0.41
4:H:125:ALA:HA	4:H:126:PRO:HD3	1.95	0.41
3:G:112:ALA:HA	3:G:113:PRO:HD2	1.81	0.41
2:B:100:LEU:HD21	2:B:118:LEU:HB2	2.02	0.41
1:A:257:THR:C	1:A:259:LEU:H	2.23	0.41
1:E:123:THR:HG23	1:E:426:MET:CE	2.50	0.41
1:E:363:PRO:HB2	5:E:862:NAG:C8	2.51	0.41
2:B:131:ARG:HG3	2:B:135:GLY:HA2	2.02	0.41
1:A:215:ILE:HD12	1:A:253:PRO:CG	2.48	0.41
1:E:119:CYS:CB	4:H:100(I):MET:HG3	2.50	0.41
1:E:117:LYS:HA	1:E:118:PRO:HD3	1.71	0.41
1:E:281:ALA:HB2	2:F:29:LYS:NZ	2.35	0.41
1:A:457:ASP:OD1	1:A:457:ASP:N	2.54	0.41
4:D:207:VAL:HG12	4:D:209:LYS:H	1.86	0.41
1:A:307:ILE:HD11	1:E:213:ILE:HD13	2.03	0.41
1:A:304:ARG:HG3	1:A:323:ILE:HD13	2.01	0.41
1:A:272:ILE:CG2	1:A:286:VAL:HG22	2.34	0.41
1:E:390:LEU:HD21	1:E:416:LEU:HD22	2.03	0.41
1:A:375:SER:O	1:A:376:PHE:HB3	2.20	0.41
1:A:286:VAL:HG11	1:A:345:ILE:HD13	2.03	0.41
1:E:276:ASN:HD22	1:E:279:ASN:HB2	1.84	0.41
1:A:281:ALA:HB1	2:B:27:HIS:CD2	2.56	0.41
2:F:128:VAL:CG1	2:F:144:LEU:HD12	2.50	0.41
1:A:305:LYS:HA	1:A:320:THR:O	2.21	0.41
4:H:195:ILE:HD12	4:H:195:ILE:N	2.35	0.41
3:C:203:SER:HA	3:C:204:PRO:HD3	1.85	0.41
1:A:365:SER:HA	5:A:862:NAG:H83	2.03	0.41
1:E:427:TRP:CE2	1:E:428:GLN:HG3	2.56	0.41
2:F:12:VAL:HG22	2:F:13:GLU:H	1.85	0.41
3:G:82:ASP:O	3:G:104:LEU:HD13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:36:TRP:HD1	4:D:69:ILE:HD13	1.85	0.41
3:G:35:TRP:CG	3:G:73:LEU:HD13	2.56	0.40
1:E:295:ASN:O	1:E:331:CYS:HA	2.22	0.40
3:G:43:ALA:HA	3:G:44:PRO:HD3	1.96	0.40
1:A:490:LYS:HG2	1:A:492:GLU:HG3	2.03	0.40
3:C:83:PHE:CE1	3:C:106:ILE:HG12	2.57	0.40
4:D:94:SER:HA	4:D:95:PRO:HD3	1.94	0.40
1:A:371:ILE:HD11	2:B:43:PHE:HB2	2.03	0.40
4:D:148:GLU:HG2	4:D:176:TYR:CE2	2.56	0.40
4:D:200:HIS:CE1	4:D:202:PRO:HB2	2.56	0.40
2:F:125:SER:HA	2:F:126:PRO:HD2	1.79	0.40
2:F:132:SER:HB2	2:F:133:PRO:CD	2.52	0.40
1:E:95:MET:HE1	1:E:235:GLY:HA3	2.03	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	315/322 (98%)	275 (87%)	34 (11%)	6 (2%)	10	45
1	E	308/322 (96%)	270 (88%)	32 (10%)	6 (2%)	10	45
2	B	176/181 (97%)	152 (86%)	20 (11%)	4 (2%)	8	39
2	F	177/181 (98%)	152 (86%)	20 (11%)	5 (3%)	6	34
3	C	211/214 (99%)	176 (83%)	30 (14%)	5 (2%)	7	38
3	G	211/214 (99%)	174 (82%)	32 (15%)	5 (2%)	7	38
4	D	227/231 (98%)	185 (82%)	37 (16%)	5 (2%)	8	41
4	H	227/231 (98%)	184 (81%)	38 (17%)	5 (2%)	8	41
All	All	1852/1896 (98%)	1568 (85%)	243 (13%)	41 (2%)	8	41

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	147	SER
4	D	2	VAL
4	D	150	VAL
2	F	147	SER
4	H	2	VAL
4	H	150	VAL
1	A	386	ASN
3	C	76	SER
4	D	173	SER
1	E	386	ASN
4	H	173	SER
1	A	116	LEU
1	A	374	HIS
1	A	464	GLY
2	B	19	SER
4	D	133	GLY
4	D	200	HIS
1	E	116	LEU
1	E	374	HIS
1	E	464	GLY
2	F	19	SER
2	F	178	ALA
3	G	76	SER
4	H	133	GLY
4	H	200	HIS
1	A	120	VAL
3	C	127	SER
3	C	138	ASN
3	G	127	SER
3	G	138	ASN
1	A	461	ASP
3	C	128	GLY
1	E	120	VAL
1	E	461	ASP
3	G	128	GLY
2	B	141	GLY
2	F	141	GLY
2	B	123	GLY
3	C	157	GLY
2	F	123	GLY
3	G	157	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	281/285 (99%)	271 (96%)	10 (4%)	42	76
1	E	276/285 (97%)	260 (94%)	16 (6%)	25	64
2	B	161/164 (98%)	157 (98%)	4 (2%)	55	82
2	F	162/164 (99%)	159 (98%)	3 (2%)	65	85
3	C	188/189 (100%)	183 (97%)	5 (3%)	52	81
3	G	188/189 (100%)	180 (96%)	8 (4%)	35	72
4	D	192/192 (100%)	190 (99%)	2 (1%)	82	91
4	H	192/192 (100%)	189 (98%)	3 (2%)	70	87
All	All	1640/1660 (99%)	1589 (97%)	51 (3%)	47	79

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	234	ASN
1	A	249	HIS
1	A	270	ILE
1	A	300	ASN
1	A	328	GLN
1	A	334	SER
1	A	372	VAL
1	A	386	ASN
1	A	452	LEU
1	A	465	THR
2	B	51	LEU
2	B	74	LEU
2	B	109	LEU
2	B	177	LEU
3	C	47	LEU
3	C	50	LYS
3	C	72	THR
3	C	132	VAL
3	C	158	ASN

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Mol	Chain	Res	Type
4	D	59	TYR
4	D	149	PRO
1	E	119	CYS
1	E	234	ASN
1	E	243	SER
1	E	249	HIS
1	E	270	ILE
1	E	300	ASN
1	E	328	GLN
1	E	334	SER
1	E	352	GLN
1	E	393	TRP
1	E	394	ASN
1	E	416	LEU
1	E	447	SER
1	E	452	LEU
1	E	456	ARG
1	E	465	THR
2	F	51	LEU
2	F	74	LEU
2	F	177	LEU
3	G	47	LEU
3	G	72	THR
3	G	90	GLN
3	G	132	VAL
3	G	148	TRP
3	G	155	GLN
3	G	211	ARG
3	G	213	GLU
4	H	59	TYR
4	H	80	MET
4	H	83	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
1	A	249	HIS
1	A	308	ASN
1	A	328	GLN
1	A	330	HIS
1	A	340	ASN

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Mol	Chain	Res	Type
1	A	389	GLN
2	B	27	HIS
2	B	32	ASN
2	B	40	GLN
3	C	3	GLN
3	C	6	GLN
3	C	38	GLN
3	C	79	GLN
3	C	90	GLN
3	C	137	ASN
3	C	189	HIS
4	D	58	HIS
4	D	61	GLN
1	E	99	ASN
1	E	229	ASN
1	E	249	HIS
1	E	308	ASN
1	E	328	GLN
1	E	340	ASN
1	E	389	GLN
2	F	27	HIS
2	F	66	ASN
3	G	6	GLN
3	G	37	GLN
3	G	38	GLN
3	G	79	GLN
3	G	124	GLN
3	G	137	ASN
4	H	58	HIS
4	H	61	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	TYS	D	100	4	15,16,17	1.11	2 (13%)	16,22,24	0.87	1 (6%)
4	TYS	D	100(C)	4	15,16,17	1.11	1 (6%)	16,22,24	0.92	1 (6%)
4	TYS	H	100	4	15,16,17	1.11	3 (20%)	16,22,24	0.86	1 (6%)
4	TYS	H	100(C)	4	15,16,17	1.10	1 (6%)	16,22,24	0.92	1 (6%)

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	TYS	D	100	4	-	0/9/11/13	0/1/1/1
4	TYS	D	100(C)	4	-	0/9/11/13	0/1/1/1
4	TYS	H	100	4	-	0/9/11/13	0/1/1/1
4	TYS	H	100(C)	4	-	0/9/11/13	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	100(C)	TYS	OH-CZ	-2.78	1.38	1.42
4	H	100(C)	TYS	OH-CZ	-2.75	1.38	1.42
4	D	100	TYS	OH-CZ	-2.53	1.38	1.42
4	H	100	TYS	OH-CZ	-2.51	1.38	1.42
4	H	100	TYS	O2-S	2.01	1.52	1.45
4	H	100	TYS	O1-S	2.06	1.52	1.45
4	D	100	TYS	O1-S	2.09	1.52	1.45

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	100(C)	TYS	CZ-OH-S	-2.95	113.49	118.52
4	H	100(C)	TYS	CZ-OH-S	-2.95	113.49	118.52
4	D	100	TYS	CZ-OH-S	-2.41	114.41	118.52
4	H	100	TYS	CZ-OH-S	-2.39	114.44	118.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	100	TYS	1	0
4	D	100(C)	TYS	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

42 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	$\#\|Z\| > 2$
6	MLA	A	3	-	0,6,6	0.00	-	0,7,7	0.00	-
5	NAG	A	734	1	14,14,15	0.50	0	15,19,21	0.69	0
5	NAG	A	741	1	14,14,15	0.60	0	15,19,21	1.47	1 (6%)
5	NAG	A	762	1	14,14,15	0.47	0	15,19,21	1.19	1 (6%)
5	NAG	A	776	1	14,14,15	0.47	0	15,19,21	1.01	2 (13%)
5	NAG	A	789	1	14,14,15	0.50	0	15,19,21	0.82	1 (6%)
5	NAG	A	795	1	14,14,15	0.53	0	15,19,21	0.66	0
7	EDO	A	8	-	3,3,3	0.46	0	2,2,2	0.40	0
5	NAG	A	801	1	14,14,15	0.49	0	15,19,21	0.67	0
5	NAG	A	832	1	14,14,15	0.48	0	15,19,21	1.09	1 (6%)
5	NAG	A	856	1	14,14,15	0.46	0	15,19,21	0.64	0
5	NAG	A	862	1	14,14,15	0.67	0	15,19,21	1.47	2 (13%)
5	NAG	A	886	1	14,14,15	0.45	0	15,19,21	1.23	2 (13%)
5	NAG	A	894	1	14,14,15	0.40	0	15,19,21	1.12	1 (6%)
5	NAG	A	900	1	14,14,15	0.46	0	15,19,21	1.11	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	A	913	1	14,14,15	0.48	0	15,19,21	0.96	1 (6%)
5	NAG	A	948	1	14,14,15	0.51	0	15,19,21	0.60	0
5	NAG	A	963	1	14,14,15	0.45	0	15,19,21	1.24	1 (6%)
6	MLA	B	186	-	0,6,6	0.00	-	0,7,7	0.00	-
7	EDO	C	215	-	3,3,3	0.47	0	2,2,2	0.36	0
7	EDO	C	216	-	3,3,3	0.47	0	2,2,2	0.40	0
7	EDO	D	215	-	3,3,3	0.49	0	2,2,2	0.23	0
7	EDO	E	10	-	3,3,3	0.48	0	2,2,2	0.38	0
7	EDO	E	7	-	3,3,3	0.45	0	2,2,2	0.47	0
5	NAG	E	734	1	14,14,15	0.50	0	15,19,21	0.74	1 (6%)
5	NAG	E	741	1	14,14,15	0.47	0	15,19,21	0.68	0
5	NAG	E	762	1	14,14,15	0.46	0	15,19,21	1.12	1 (6%)
5	NAG	E	776	1	14,14,15	0.47	0	15,19,21	1.63	1 (6%)
5	NAG	E	789	1	14,14,15	0.47	0	15,19,21	0.70	0
5	NAG	E	795	1	14,14,15	0.50	0	15,19,21	0.61	0
5	NAG	E	801	1	14,14,15	0.47	0	15,19,21	1.23	1 (6%)
5	NAG	E	832	1	14,14,15	0.54	0	15,19,21	0.72	0
5	NAG	E	856	1	14,14,15	0.50	0	15,19,21	0.73	0
5	NAG	E	862	1	14,14,15	0.47	0	15,19,21	1.16	1 (6%)
5	NAG	E	886	1	14,14,15	0.52	0	15,19,21	0.76	0
5	NAG	E	894	1	14,14,15	0.54	0	15,19,21	1.32	1 (6%)
5	NAG	E	913	1	14,14,15	0.50	0	15,19,21	1.18	1 (6%)
5	NAG	E	948	1	14,14,15	0.48	0	15,19,21	0.77	0
5	NAG	E	963	1	14,14,15	0.57	0	15,19,21	1.00	1 (6%)
6	MLA	F	186	-	0,6,6	0.00	-	0,7,7	0.00	-
7	EDO	F	187	-	3,3,3	0.48	0	2,2,2	0.33	0
6	MLA	H	215	-	0,6,6	0.00	-	0,7,7	0.00	-

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	MLA	A	3	-	-	0/0/4/4	0/0/0/0
5	NAG	A	734	1	-	0/6/23/26	0/1/1/1
5	NAG	A	741	1	-	0/6/23/26	0/1/1/1
5	NAG	A	762	1	-	0/6/23/26	0/1/1/1
5	NAG	A	776	1	-	0/6/23/26	0/1/1/1
5	NAG	A	789	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	795	1	-	0/6/23/26	0/1/1/1
7	EDO	A	8	-	-	0/1/1/1	0/0/0/0
5	NAG	A	801	1	-	2/6/23/26	0/1/1/1
5	NAG	A	832	1	-	1/6/23/26	0/1/1/1
5	NAG	A	856	1	-	0/6/23/26	0/1/1/1
5	NAG	A	862	1	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	A	886	1	-	0/6/23/26	0/1/1/1
5	NAG	A	894	1	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	A	900	1	-	1/6/23/26	0/1/1/1
5	NAG	A	913	1	-	0/6/23/26	0/1/1/1
5	NAG	A	948	1	-	0/6/23/26	0/1/1/1
5	NAG	A	963	1	-	0/6/23/26	0/1/1/1
6	MLA	B	186	-	-	0/0/4/4	0/0/0/0
7	EDO	C	215	-	-	0/1/1/1	0/0/0/0
7	EDO	C	216	-	-	0/1/1/1	0/0/0/0
7	EDO	D	215	-	-	0/1/1/1	0/0/0/0
7	EDO	E	10	-	-	0/1/1/1	0/0/0/0
7	EDO	E	7	-	-	0/1/1/1	0/0/0/0
5	NAG	E	734	1	-	0/6/23/26	0/1/1/1
5	NAG	E	741	1	-	0/6/23/26	0/1/1/1
5	NAG	E	762	1	-	0/6/23/26	0/1/1/1
5	NAG	E	776	1	-	0/6/23/26	0/1/1/1
5	NAG	E	789	1	-	0/6/23/26	0/1/1/1
5	NAG	E	795	1	-	0/6/23/26	0/1/1/1
5	NAG	E	801	1	-	0/6/23/26	0/1/1/1
5	NAG	E	832	1	-	0/6/23/26	0/1/1/1
5	NAG	E	856	1	-	0/6/23/26	0/1/1/1
5	NAG	E	862	1	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	E	886	1	-	0/6/23/26	0/1/1/1
5	NAG	E	894	1	-	0/6/23/26	0/1/1/1
5	NAG	E	913	1	-	2/6/23/26	0/1/1/1
5	NAG	E	948	1	-	0/6/23/26	0/1/1/1
5	NAG	E	963	1	1/1/5/7	0/6/23/26	0/1/1/1
6	MLA	F	186	-	-	0/0/4/4	0/0/0/0
7	EDO	F	187	-	-	0/1/1/1	0/0/0/0
6	MLA	H	215	-	-	0/0/4/4	0/0/0/0

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	886	NAG	C2-N2-C7	-2.25	120.14	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	862	NAG	C2-N2-C7	-2.22	120.18	123.04
5	A	900	NAG	C6-C5-C4	-2.12	107.77	113.02
5	A	776	NAG	C2-N2-C7	-2.07	120.38	123.04
5	E	734	NAG	C1-O5-C5	2.16	114.98	112.25
5	A	789	NAG	C1-O5-C5	2.23	115.07	112.25
5	E	963	NAG	C1-O5-C5	2.26	115.12	112.25
5	A	900	NAG	C3-C4-C5	2.27	114.16	110.20
5	A	776	NAG	C1-O5-C5	2.79	115.78	112.25
5	A	913	NAG	C1-O5-C5	3.04	116.10	112.25
5	E	762	NAG	C1-O5-C5	3.23	116.35	112.25
5	A	894	NAG	C1-O5-C5	3.44	116.61	112.25
5	A	762	NAG	C1-O5-C5	3.60	116.81	112.25
5	A	832	NAG	C1-O5-C5	3.60	116.82	112.25
5	A	886	NAG	C1-O5-C5	3.64	116.86	112.25
5	E	862	NAG	C1-O5-C5	3.74	116.99	112.25
5	E	913	NAG	C1-O5-C5	3.97	117.29	112.25
5	A	963	NAG	C1-O5-C5	4.38	117.80	112.25
5	E	894	NAG	C1-O5-C5	4.40	117.83	112.25
5	A	862	NAG	C1-O5-C5	4.41	117.84	112.25
5	E	801	NAG	C1-O5-C5	4.42	117.86	112.25
5	A	741	NAG	C1-O5-C5	5.17	118.81	112.25
5	E	776	NAG	C1-O5-C5	5.52	119.25	112.25

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	862	NAG	C1
5	E	862	NAG	C1
5	E	963	NAG	C1
5	A	894	NAG	C1

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	900	NAG	O7-C7-N2-C2
5	A	832	NAG	O7-C7-N2-C2
5	A	801	NAG	C8-C7-N2-C2
5	E	913	NAG	O7-C7-N2-C2
5	A	801	NAG	O7-C7-N2-C2
5	E	913	NAG	C8-C7-N2-C2

There are no ring outliers.

13 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	734	NAG	1	0
5	A	776	NAG	2	0
5	A	789	NAG	1	0
5	A	832	NAG	1	0
5	A	862	NAG	2	0
5	A	894	NAG	4	0
5	A	913	NAG	1	0
5	A	963	NAG	1	0
7	E	7	EDO	1	0
5	E	762	NAG	1	0
5	E	789	NAG	3	0
5	E	862	NAG	1	0
5	E	913	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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	319/322 (99%)	0.04	5 (1%) 74 69	75, 116, 185, 255	0
1	E	312/322 (96%)	0.01	3 (0%) 84 80	81, 118, 177, 236	0
2	B	178/181 (98%)	0.12	7 (3%) 43 36	95, 163, 213, 229	0
2	F	179/181 (98%)	0.24	12 (6%) 21 17	96, 163, 213, 228	0
3	C	213/214 (99%)	0.51	26 (12%) 5 4	104, 189, 260, 275	0
3	G	213/214 (99%)	0.92	46 (21%) 1 1	103, 195, 262, 275	0
4	D	229/231 (99%)	0.40	19 (8%) 14 11	92, 157, 259, 288	0
4	H	229/231 (99%)	0.49	23 (10%) 9 8	97, 157, 265, 289	0
All	All	1872/1896 (98%)	0.31	141 (7%) 17 14	75, 147, 250, 289	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	114	SER	10.6
3	G	197	THR	10.3
4	D	125	ALA	7.9
3	C	115	VAL	7.6
2	F	142	LYS	7.6
4	H	183	THR	7.4
3	G	203	SER	6.9
4	D	159	LEU	6.6
3	G	202	SER	6.5
3	G	145	LYS	6.4
3	C	134	CYS	6.2
4	H	136	ALA	5.9
4	H	123	PRO	5.7
3	G	115	VAL	5.6
4	H	137	ALA	5.6
4	D	138	LEU	5.4

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Mol	Chain	Res	Type	RSRZ
4	H	126	PRO	5.3
3	G	196	VAL	5.3
3	G	176	SER	5.1
3	C	197	THR	5.1
4	D	194	TYR	5.0
4	H	138	LEU	4.9
3	G	193	ALA	4.9
3	G	150	VAL	4.7
4	H	181	VAL	4.5
3	G	209	PHE	4.4
3	G	198	HIS	4.4
3	G	181	LEU	4.3
3	G	113	PRO	4.3
4	D	124	LEU	4.2
3	C	131	SER	4.2
4	D	181	VAL	4.2
3	G	144	ALA	4.1
4	H	139	GLY	4.1
4	H	184	VAL	4.1
1	E	359	ILE	4.1
4	D	184	VAL	4.0
3	G	208	SER	4.0
4	D	180	SER	3.9
4	D	182	VAL	3.8
3	G	135	LEU	3.8
4	H	182	VAL	3.8
2	F	145	SER	3.7
3	G	175	LEU	3.7
3	C	208	SER	3.7
4	H	124	LEU	3.6
4	D	139	GLY	3.6
3	C	186	TYR	3.6
3	C	133	VAL	3.6
2	F	98	PHE	3.6
3	G	148	TRP	3.6
2	F	139	GLN	3.5
3	G	146	VAL	3.5
3	G	189	HIS	3.5
4	D	136	ALA	3.5
4	D	179	SER	3.5
4	H	194	TYR	3.5
3	G	134	CYS	3.4

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Mol	Chain	Res	Type	RSRZ
3	G	47	LEU	3.4
3	C	132	VAL	3.4
1	A	403	GLY	3.4
1	A	402	THR	3.4
2	B	118	LEU	3.3
3	G	192	TYR	3.3
3	G	205	VAL	3.3
3	C	116	PHE	3.3
3	G	149	LYS	3.3
3	G	133	VAL	3.2
2	F	118	LEU	3.2
3	G	199	GLN	3.2
4	D	140	CYS	3.2
2	F	143	THR	3.1
3	G	131	SER	3.1
4	H	127	SER	3.1
4	H	141	LEU	3.1
4	H	212	GLU	3.1
4	H	140	CYS	3.0
4	D	208	ASP	3.0
2	F	179	PHE	3.0
3	C	175	LEU	3.0
4	D	142	VAL	3.0
3	C	73	LEU	3.0
4	D	82	LEU	3.0
3	G	118	PHE	2.9
3	G	165	GLU	2.9
3	C	144	ALA	2.9
3	C	213	GLU	2.9
3	C	152	ASN	2.9
3	G	190	LYS	2.9
3	G	195	GLU	2.9
2	B	98	PHE	2.8
2	F	116	LEU	2.8
3	C	114	SER	2.8
3	G	117	ILE	2.8
3	C	128	GLY	2.8
2	F	144	LEU	2.8
2	B	14	LEU	2.7
2	B	116	LEU	2.7
3	G	151	ASP	2.7
2	F	146	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	108	LEU	2.7
3	C	189	HIS	2.7
4	H	121	VAL	2.7
4	D	193	THR	2.6
3	G	182	SER	2.6
3	C	180	THR	2.6
3	G	116	PHE	2.6
3	G	62	PHE	2.6
4	H	198	VAL	2.6
3	G	136	LEU	2.5
3	C	151	ASP	2.5
3	C	177	SER	2.5
3	C	117	ILE	2.4
4	H	185	PRO	2.4
4	H	180	SER	2.4
3	G	187	GLU	2.4
3	C	148	TRP	2.4
3	C	156	SER	2.4
2	F	173	ASP	2.4
1	A	391	PHE	2.3
1	E	391	PHE	2.3
4	H	213	PRO	2.3
4	D	121	VAL	2.3
2	F	141	GLY	2.3
3	C	149	LYS	2.3
2	B	5	LEU	2.3
3	C	159	SER	2.3
1	A	361	PHE	2.3
3	G	201	LEU	2.3
3	G	132	VAL	2.3
2	B	115	THR	2.3
3	C	209	PHE	2.3
1	E	361	PHE	2.2
4	H	125	ALA	2.2
3	G	180	THR	2.2
3	G	186	TYR	2.2
3	G	206	THR	2.2
1	A	350	LYS	2.1
3	G	156	SER	2.1
4	H	101	ASP	2.1
4	D	148	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	TYS	H	100	16/17	0.95	0.19	-	129,148,162,171	0
4	TYS	H	100(C)	16/17	0.97	0.19	-	97,111,132,175	0
4	TYS	D	100	16/17	0.95	0.22	-	130,143,158,167	0
4	TYS	D	100(C)	16/17	0.97	0.19	-	94,108,129,177	0

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	NAG	A	900	14/15	0.54	1.38	9.83	261,310,326,329	0
5	NAG	A	894	14/15	0.51	0.83	4.85	222,258,266,268	0
5	NAG	E	832	14/15	0.88	0.24	3.35	138,157,187,188	0
5	NAG	A	832	14/15	0.91	0.24	3.10	145,167,199,205	0
5	NAG	E	801	14/15	0.89	0.24	2.23	127,177,189,190	0
6	MLA	H	215	7/7	0.52	0.34	1.92	181,191,199,201	0
5	NAG	E	886	14/15	0.91	0.24	1.86	139,152,191,202	0
5	NAG	E	762	14/15	0.94	0.26	0.51	88,103,115,119	0
5	NAG	A	762	14/15	0.95	0.25	0.14	73,97,118,127	0
5	NAG	E	795	14/15	0.93	0.18	0.04	119,138,146,153	0
5	NAG	A	913	14/15	0.79	0.25	-0.13	164,196,225,227	0
5	NAG	E	776	14/15	0.90	0.16	-0.16	128,140,175,175	0
5	NAG	A	795	14/15	0.96	0.17	-0.54	89,122,133,145	0
5	NAG	E	963	14/15	0.58	0.45	-0.64	257,278,307,314	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	NAG	A	886	14/15	0.92	0.18	-0.71	131,151,182,189	0
5	NAG	E	789	14/15	0.93	0.14	-1.32	151,182,197,203	0
5	NAG	A	789	14/15	0.89	0.15	-1.52	132,155,165,166	0
5	NAG	E	948	14/15	0.91	0.20	-	116,153,161,163	0
5	NAG	A	856	14/15	0.55	0.56	-	215,243,260,271	0
5	NAG	E	894	14/15	0.68	0.65	-	242,252,258,260	0
5	NAG	E	734	14/15	0.88	0.20	-	200,219,224,226	0
5	NAG	A	734	14/15	0.91	0.17	-	192,222,231,236	0
5	NAG	A	963	14/15	0.55	0.76	-	249,284,309,310	0
7	EDO	C	215	4/4	0.88	0.33	-	122,127,130,130	0
5	NAG	A	801	14/15	0.90	0.21	-	134,181,187,191	0
5	NAG	E	862	14/15	0.62	1.09	-	208,248,258,260	0
5	NAG	A	741	14/15	0.88	0.30	-	194,213,222,225	0
5	NAG	E	741	14/15	0.88	0.40	-	192,220,234,236	0
6	MLA	B	186	7/7	0.72	0.34	-	177,181,190,190	0
7	EDO	C	216	4/4	0.76	0.45	-	148,156,166,167	0
7	EDO	E	10	4/4	0.86	0.18	-	130,139,140,143	0
7	EDO	E	7	4/4	0.90	0.26	-	127,135,139,146	0
7	EDO	D	215	4/4	0.93	0.16	-	100,106,111,111	0
5	NAG	A	776	14/15	0.89	0.17	-	137,161,180,185	0
5	NAG	E	856	14/15	0.37	0.45	-	242,258,275,275	0
7	EDO	F	187	4/4	0.69	0.51	-	127,128,135,140	0
5	NAG	A	862	14/15	0.70	0.67	-	214,228,244,250	0
5	NAG	E	913	14/15	0.74	0.26	-	226,244,266,268	0
6	MLA	F	186	7/7	0.54	0.28	-	180,189,200,207	0
5	NAG	A	948	14/15	0.92	0.20	-	124,141,149,156	0
7	EDO	A	8	4/4	0.90	0.31	-	153,153,154,156	0
6	MLA	A	3	7/7	0.29	0.56	-	175,186,200,209	0

6.5 Other polymers (i)

There are no such residues in this entry.