Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:11 AM GMT

PDB ID	:	2FX9
Title	:	Crystal structure of hiv-1 neutralizing human fab 4e10 in complex with a thioether-linked peptide encompassing the 4e10 epitope on gp41
Authors	:	Cardoso, R.M.F.; Brunel, F.M.; Ferguson, S.; Burton, D.R.; Dawson, P.E.; Wilson, I.A.
Deposited on	:	2006-02-03
Resolution	:	2.10 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:

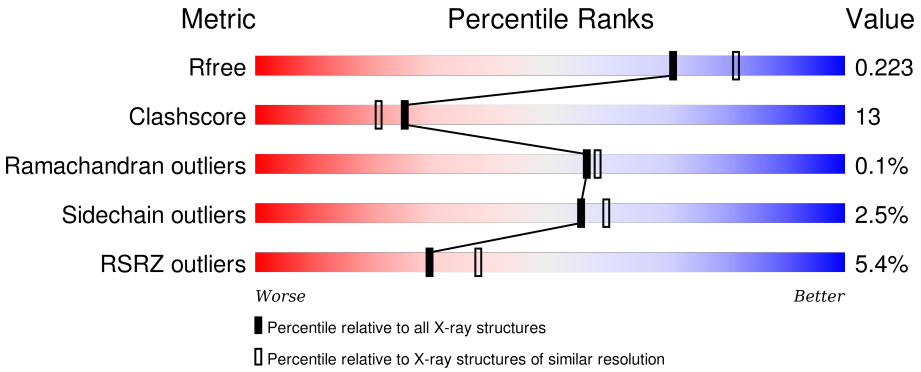
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	L	214	3% 72% 27%
1	M	214	7% 68% 31%
2	H	227	7% 79% 21%
2	I	227	4% 78% 22%
3	P	14	14% 50% 43% 7%

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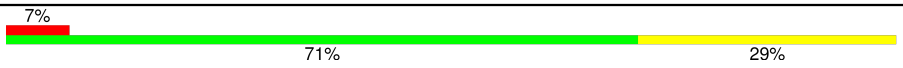
Mol	Chain	Length	Quality of chain
3	Q	14	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7319 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 Fab 4E10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	214	Total	C	N	O	S	0	0	0
			1639	1017	284	334	4			
1	M	214	Total	C	N	O	S	0	0	0
			1639	1017	284	334	4			

- Molecule 2 is a protein called Fab 4E10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	227	Total	C	N	O	S	0	0	0
			1681	1063	287	326	5			
2	I	227	Total	C	N	O	S	0	0	0
			1681	1063	287	326	5			

- Molecule 3 is a protein called Fragment of HIV glycoprotein gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	14	Total	C	N	O	S	0	0	0
			138	96	23	18	1			
3	Q	14	Total	C	N	O	S	0	0	0
			138	96	23	18	1			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	96	Total	O	0	0
			96	96		
4	H	85	Total	O	0	0
			85	85		
4	M	98	Total	O	0	0
			98	98		
4	I	113	Total	O	0	0
			113	113		

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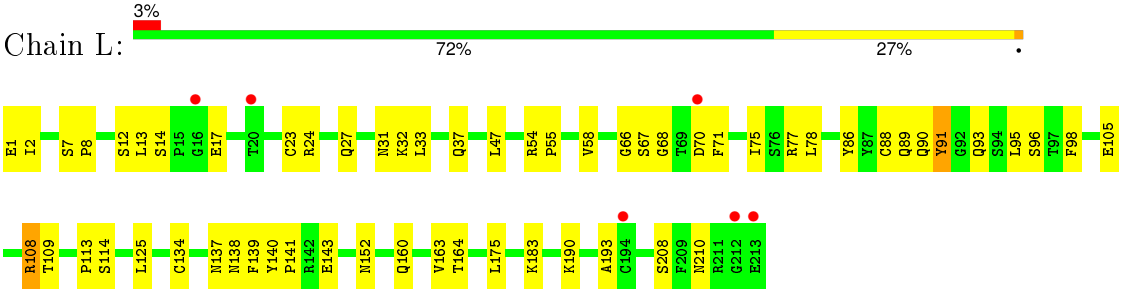
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	P	5	Total O 5 5	0	0
4	Q	6	Total O 6 6	0	0

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.

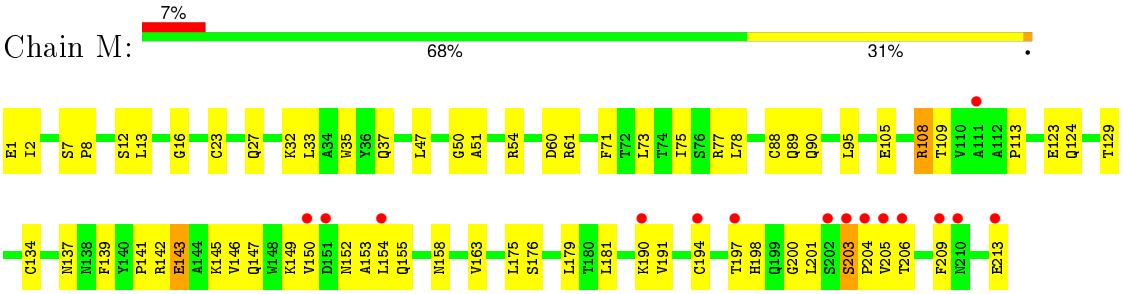
- Molecule 1: Fab 4E10

Chain L:



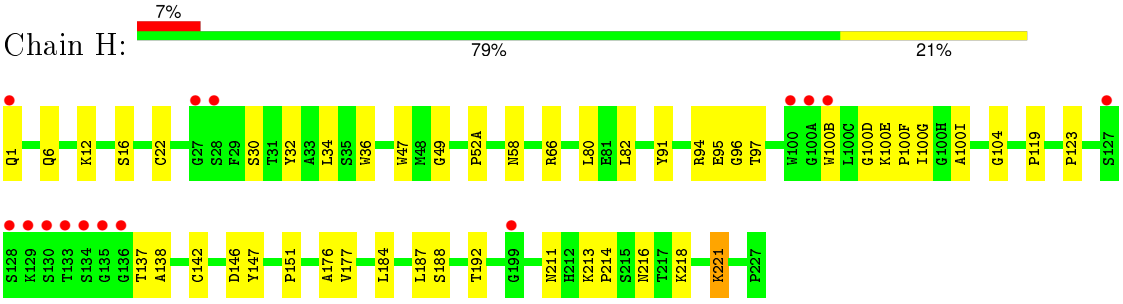
- Molecule 1: Fab 4E10

Chain M:



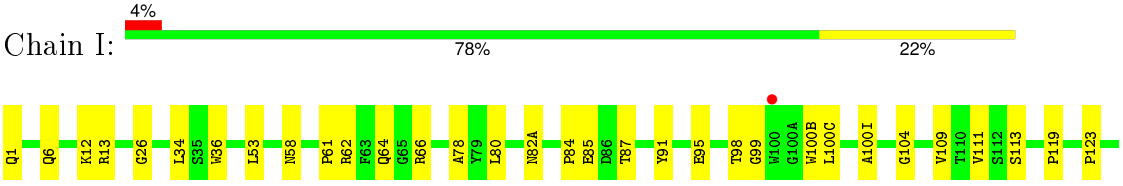
- Molecule 2: Fab 4E10

Chain H:

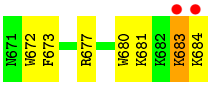


- Molecule 2: Fab 4E10

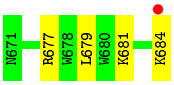
Chain I:



• Molecule 3: Fragment of HIV glycoprotein gp41



• Molecule 3: Fragment of HIV glycoprotein gp41



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	53.42Å 111.50Å 79.38Å 90.00° 106.44° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 38.07 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.00-2.10) 99.1 (38.07-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.76 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.236 , 0.271 0.234 , 0.223	Depositor DCC
R_{free} test set	2633 reflections (5.11%)	DCC
Wilson B-factor (Å^2)	28.4	Xtriage
Anisotropy	0.521	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 47.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 51545 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7319	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.84% 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: ORQ

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	L	0.44	3/1672 (0.2%)	0.62	0/2266
1	M	0.46	4/1672 (0.2%)	0.65	1/2266 (0.0%)
2	H	0.42	2/1724 (0.1%)	0.64	0/2355
2	I	0.42	2/1724 (0.1%)	0.65	0/2355
3	P	0.53	0/132	0.57	0/174
3	Q	0.59	0/132	0.61	0/174
All	All	0.44	11/7056 (0.2%)	0.64	1/9590 (0.0%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	23	CYS	CB-SG	7.04	1.94	1.82
1	M	194	CYS	CB-SG	7.03	1.94	1.82
1	L	23	CYS	CB-SG	6.72	1.93	1.82
1	M	134	CYS	CB-SG	6.44	1.93	1.82
1	L	88	CYS	CB-SG	6.32	1.93	1.82
2	I	208	CYS	CB-SG	5.94	1.92	1.82
2	I	142	CYS	CB-SG	5.84	1.92	1.82
2	H	142	CYS	CB-SG	5.72	1.92	1.82
1	L	134	CYS	CB-SG	5.63	1.91	1.82
2	H	22	CYS	CB-SG	5.42	1.91	1.82
1	M	88	CYS	CB-SG	5.17	1.91	1.82

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	203	SER	C-N-CD	5.87	140.73	128.40

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	L	1639	0	1589	39	0
1	M	1639	0	1589	56	0
2	H	1681	0	1666	34	0
2	I	1681	0	1666	39	0
3	P	138	0	139	9	0
3	Q	138	0	139	4	0
4	H	85	0	0	1	0
4	I	113	0	0	1	0
4	L	96	0	0	0	0
4	M	98	0	0	2	0
4	P	5	0	0	1	0
4	Q	6	0	0	0	0
All	All	7319	0	6788	173	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 13.

All (173) 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:H:211:ASN:HD21	2:H:218:LYS:HE2	1.32	0.93
1:M:123:GLU:HG3	4:M:286:HOH:O	1.73	0.86
1:M:158:ASN:ND2	1:M:179:LEU:HD11	1.95	0.82
2:I:62:ARG:HH11	2:I:62:ARG:HB3	1.47	0.79
2:H:119:PRO:HB3	2:H:147:TYR:HB3	1.64	0.77
2:I:119:PRO:HB3	2:I:147:TYR:HB3	1.65	0.77
1:M:154:LEU:HD12	1:M:154:LEU:O	1.84	0.76
1:M:37:GLN:HB2	1:M:47:LEU:HD11	1.68	0.75
2:H:30:SER:HA	2:H:52(A):PRO:HB2	1.69	0.74
2:I:211:ASN:ND2	2:I:218:LYS:HE2	2.03	0.73
1:M:145:LYS:HB3	1:M:197:THR:OG1	1.88	0.73
1:L:32:LYS:NZ	3:P:677:ORQ:O1	2.17	0.73
1:L:108:ARG:HD3	1:L:109:THR:O	1.88	0.72
2:I:62:ARG:HB3	2:I:62:ARG:NH1	2.05	0.70
1:M:145:LYS:HD3	1:M:147:GLN:HG3	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:113:PRO:HB3	1:M:139:PHE:HB3	1.74	0.69
1:L:33:LEU:HD22	1:L:71:PHE:CG	2.30	0.67
1:L:24:ARG:NH1	1:L:70:ASP:HB2	2.10	0.66
1:M:158:ASN:HD22	1:M:181:LEU:HD21	1.61	0.66
2:I:211:ASN:HD22	2:I:218:LYS:HE2	1.61	0.66
1:M:197:THR:HG22	1:M:204:PRO:HB3	1.78	0.66
1:L:143:GLU:H	1:L:143:GLU:CD	1.99	0.65
1:L:190:LYS:HE2	1:L:210:ASN:ND2	2.12	0.64
1:M:190:LYS:HG3	1:M:191:VAL:HG23	1.79	0.63
1:M:33:LEU:HD22	1:M:71:PHE:CG	2.34	0.62
3:P:683:LYS:HG3	3:P:684:LYS:N	2.15	0.61
2:H:187:LEU:C	2:H:187:LEU:HD12	2.20	0.61
1:M:149:LYS:HG2	1:M:154:LEU:HA	1.82	0.60
3:P:683:LYS:HG3	3:P:684:LYS:H	1.67	0.60
1:M:203:SER:O	1:M:204:PRO:C	2.35	0.59
1:M:54:ARG:NH1	1:M:60:ASP:HA	2.17	0.59
1:L:14:SER:O	1:L:17:GLU:HB2	2.01	0.58
2:I:61:PRO:HA	2:I:64:GLN:HG2	1.84	0.58
1:M:145:LYS:C	1:M:145:LYS:HD2	2.24	0.58
2:I:1:GLN:N	2:I:1:GLN:CD	2.57	0.58
1:M:32:LYS:NZ	3:Q:677:ORQ:O1	2.28	0.58
2:H:100(E):LYS:HB3	3:P:680:TRP:CE3	2.40	0.57
2:H:6:GLN:HE21	2:H:104:GLY:HA3	1.70	0.57
1:L:190:LYS:HE2	1:L:210:ASN:HD22	1.70	0.57
1:L:2:ILE:HG12	1:L:27:GLN:CG	2.34	0.57
2:H:1:GLN:O	2:H:1:GLN:HG3	2.05	0.57
1:M:158:ASN:HD21	1:M:179:LEU:HD11	1.66	0.56
2:I:205:THR:HG23	2:I:222:LYS:HE3	1.88	0.56
2:I:1:GLN:CD	2:I:1:GLN:H3	2.08	0.56
2:H:221:LYS:NZ	2:H:221:LYS:HB2	2.21	0.56
1:L:47:LEU:O	1:L:55:PRO:HD2	2.06	0.56
2:H:100(E):LYS:HB3	3:P:680:TRP:CZ3	2.41	0.55
1:L:114:SER:OG	1:L:137:ASN:HB3	2.06	0.55
2:H:146:ASP:HB3	2:H:184:LEU:HD13	1.87	0.55
1:M:142:ARG:HG2	1:M:142:ARG:HH21	1.72	0.55
2:I:34:LEU:HD13	2:I:78:ALA:HB2	1.89	0.55
1:M:152:ASN:HB2	4:M:233:HOH:O	2.06	0.54
2:I:6:GLN:HE21	2:I:104:GLY:HA3	1.72	0.54
1:M:197:THR:HG22	1:M:204:PRO:CB	2.37	0.54
1:M:108:ARG:HD3	1:M:109:THR:O	2.07	0.54
2:H:211:ASN:ND2	2:H:218:LYS:HE2	2.13	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:124:GLN:HG2	1:M:129:THR:O	2.09	0.53
1:L:89:GLN:HB2	1:L:98:PHE:CD1	2.44	0.53
1:M:16:GLY:HA2	1:M:77:ARG:HG2	1.90	0.52
2:I:53:LEU:HD23	3:Q:679:LEU:HD21	1.91	0.52
1:L:37:GLN:HB2	1:L:47:LEU:HD11	1.92	0.52
1:L:143:GLU:CD	1:L:143:GLU:N	2.63	0.51
2:I:12:LYS:O	2:I:111:VAL:HA	2.10	0.51
1:M:150:VAL:O	1:M:191:VAL:O	2.28	0.51
2:I:62:ARG:HG2	2:I:62:ARG:O	2.10	0.51
1:L:12:SER:O	1:L:13:LEU:HD23	2.10	0.51
1:L:77:ARG:O	1:L:77:ARG:HG3	2.09	0.50
3:Q:681:LYS:O	3:Q:684:LYS:HB3	2.11	0.50
1:M:213:GLU:OXT	1:M:213:GLU:HG2	2.11	0.50
2:H:119:PRO:CB	2:H:147:TYR:HB3	2.38	0.50
1:L:54:ARG:HD2	1:L:58:VAL:O	2.12	0.50
1:M:197:THR:HG22	1:M:204:PRO:HG3	1.93	0.50
1:L:193:ALA:HB2	1:L:208:SER:HB3	1.94	0.49
1:L:175:LEU:HD23	1:L:175:LEU:C	2.33	0.49
1:L:7:SER:HA	1:L:8:PRO:C	2.33	0.49
1:L:163:VAL:HG12	1:L:164:THR:O	2.12	0.49
2:I:84:PRO:HB2	2:I:85:GLU:OE2	2.11	0.49
1:M:145:LYS:HB3	1:M:197:THR:HG1	1.76	0.49
3:P:680:TRP:O	3:P:683:LYS:HG3	2.13	0.49
1:M:190:LYS:HG3	1:M:191:VAL:N	2.28	0.49
2:H:95:GLU:OE1	2:H:100(F):PRO:HB2	2.13	0.48
1:L:31:ASN:HD21	1:L:68:GLY:H	1.60	0.48
1:L:75:ILE:HG21	1:L:78:LEU:HD23	1.95	0.48
2:I:6:GLN:HE22	2:I:91:TYR:HA	1.78	0.48
1:M:197:THR:HG22	1:M:204:PRO:CG	2.44	0.48
3:Q:677:ORQ:O	3:Q:681:LYS:HG2	2.14	0.47
1:M:153:ALA:O	1:M:154:LEU:C	2.51	0.47
2:I:34:LEU:C	2:I:34:LEU:HD23	2.35	0.47
2:I:187:LEU:C	2:I:187:LEU:HD12	2.34	0.47
2:H:123:PRO:HD3	2:H:221:LYS:HD3	1.95	0.47
1:M:141:PRO:O	1:M:198:HIS:HE1	1.97	0.47
2:I:176:ALA:HA	2:I:187:LEU:HB3	1.96	0.47
2:I:62:ARG:NH1	2:I:62:ARG:CB	2.76	0.47
2:H:137:THR:HG21	2:H:192:THR:HB	1.97	0.47
1:M:149:LYS:HG2	1:M:154:LEU:CA	2.44	0.47
2:I:133:THR:O	2:I:133:THR:HG22	2.15	0.47
2:H:97:THR:HG21	2:H:100(B):TRP:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:163:VAL:HG22	1:L:175:LEU:HB2	1.97	0.46
1:M:201:LEU:HD13	1:M:205:VAL:HG23	1.98	0.46
1:L:2:ILE:HG13	1:L:93:GLN:OE1	2.15	0.46
1:L:89:GLN:HG2	1:L:90:GLN:N	2.29	0.46
2:H:97:THR:OG1	2:H:100(B):TRP:HA	2.16	0.46
2:I:62:ARG:HD3	4:I:244:HOH:O	2.16	0.46
2:H:95:GLU:HA	2:H:100(I):ALA:O	2.16	0.46
1:L:125:LEU:O	1:L:183:LYS:HD2	2.16	0.46
2:I:66:ARG:HD2	2:I:82(A):ASN:O	2.16	0.45
2:H:36:TRP:CE2	2:H:80:LEU:HB2	2.51	0.45
2:H:12:LYS:HB3	2:H:16:SER:OG	2.16	0.45
1:M:145:LYS:HD2	1:M:146:VAL:N	2.32	0.45
1:M:89:GLN:HG2	1:M:90:GLN:N	2.31	0.45
2:I:87:THR:HA	2:I:109:VAL:O	2.16	0.45
1:M:61:ARG:O	1:M:75:ILE:HA	2.17	0.45
1:M:143:GLU:N	1:M:143:GLU:OE1	2.50	0.44
1:M:198:HIS:CD2	1:M:200:GLY:H	2.35	0.44
1:M:205:VAL:HG12	1:M:206:THR:N	2.32	0.44
1:M:175:LEU:HD23	1:M:176:SER:N	2.33	0.44
1:M:7:SER:HA	1:M:8:PRO:C	2.38	0.44
1:L:2:ILE:HG12	1:L:27:GLN:HG2	1.99	0.44
2:I:1:GLN:HA	2:I:100(B):TRP:CE2	2.52	0.44
2:H:58:ASN:HB2	3:P:672:TRP:CD1	2.53	0.44
2:H:96:GLY:O	2:H:100(G):ILE:HG12	2.18	0.43
2:H:32:TYR:HB3	2:H:94:ARG:HD3	2.00	0.43
1:L:113:PRO:HB3	1:L:139:PHE:HB3	2.00	0.43
2:H:137:THR:HG22	2:H:138:ALA:N	2.34	0.43
2:H:66:ARG:NH2	2:H:82:LEU:HD21	2.33	0.43
2:I:128:SER:HA	2:I:133:THR:OG1	2.18	0.43
1:L:67:SER:HA	1:L:71:PHE:CE1	2.54	0.43
2:I:1:GLN:O	2:I:26:GLY:HA3	2.19	0.43
1:M:163:VAL:HG22	1:M:175:LEU:HD12	2.00	0.43
2:I:123:PRO:HD3	2:I:221:LYS:HD3	2.00	0.43
1:L:91:TYR:CD1	1:L:91:TYR:N	2.87	0.43
2:I:36:TRP:CE2	2:I:80:LEU:HB2	2.53	0.43
1:M:155:GLN:HB3	1:M:158:ASN:OD1	2.19	0.42
2:H:187:LEU:HD12	2:H:188:SER:N	2.34	0.42
1:M:16:GLY:HA2	1:M:77:ARG:CG	2.50	0.42
1:M:12:SER:O	1:M:13:LEU:HD23	2.20	0.42
1:M:145:LYS:C	1:M:145:LYS:CD	2.88	0.42
2:I:85:GLU:CD	2:I:85:GLU:N	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:35:TRP:CD2	1:M:73:LEU:HB2	2.54	0.42
1:M:113:PRO:HD3	1:M:198:HIS:CD2	2.55	0.42
2:H:6:GLN:HE22	2:H:91:TYR:HA	1.85	0.42
2:I:13:ARG:HH22	2:I:113:SER:C	2.23	0.42
2:I:85:GLU:CD	2:I:85:GLU:H	2.23	0.42
1:M:158:ASN:ND2	1:M:179:LEU:CD1	2.75	0.42
3:P:681:LYS:HD2	4:P:391:HOH:O	2.20	0.42
2:I:141:GLY:HA2	2:I:157:TRP:CH2	2.55	0.42
1:M:50:GLY:O	1:M:51:ALA:HB3	2.20	0.42
2:I:98:THR:HG22	2:I:99:GLY:N	2.34	0.41
2:I:61:PRO:HA	2:I:64:GLN:CG	2.48	0.41
1:L:33:LEU:HD22	1:L:71:PHE:CB	2.51	0.41
1:M:142:ARG:HG2	1:M:142:ARG:NH2	2.34	0.41
1:M:209:PHE:C	1:M:209:PHE:CD1	2.94	0.41
1:L:140:TYR:CG	1:L:141:PRO:HA	2.56	0.41
1:L:163:VAL:CG2	1:L:175:LEU:HD12	2.51	0.41
1:M:75:ILE:HG21	1:M:78:LEU:HD23	2.03	0.41
1:M:190:LYS:HG3	1:M:191:VAL:H	1.86	0.41
1:L:47:LEU:HD11	1:L:86:TYR:HE1	1.86	0.41
1:L:89:GLN:HB2	1:L:98:PHE:CE1	2.55	0.41
1:M:35:TRP:CE2	1:M:73:LEU:HB2	2.56	0.41
2:H:213:LYS:N	2:H:214:PRO:CD	2.83	0.41
1:L:96:SER:HB2	3:P:673:PHE:CE1	2.56	0.41
1:L:66:GLY:HA3	1:L:71:PHE:HA	2.03	0.40
2:H:100(D):GLY:HA3	4:H:300:HOH:O	2.20	0.40
2:I:1:GLN:N	2:I:1:GLN:NE2	2.68	0.40
1:M:2:ILE:HG12	1:M:27:GLN:HG3	2.03	0.40
1:L:160:GLN:OE1	2:H:177:VAL:HG21	2.22	0.40
2:H:216:ASN:HD22	2:H:216:ASN:HA	1.71	0.40
2:H:176:ALA:HA	2:H:187:LEU:HB3	2.03	0.40
2:I:100(B):TRP:O	2:I:100(C):LEU:HD23	2.22	0.40
2:I:95:GLU:HA	2:I:100(I):ALA:O	2.22	0.40
2:I:212:HIS:CD2	2:I:214:PRO:HD2	2.56	0.40
2:H:47:TRP:CH2	2:H:49:GLY:HA2	2.56	0.40
2:H:34:LEU:C	2:H:34:LEU:HD23	2.42	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	L	212/214 (99%)	205 (97%)	6 (3%)	1 (0%)	34 30
1	M	212/214 (99%)	198 (93%)	14 (7%)	0	100 100
2	H	225/227 (99%)	215 (96%)	10 (4%)	0	100 100
2	I	225/227 (99%)	213 (95%)	12 (5%)	0	100 100
3	P	11/14 (79%)	11 (100%)	0	0	100 100
3	Q	11/14 (79%)	10 (91%)	1 (9%)	0	100 100
All	All	896/910 (98%)	852 (95%)	43 (5%)	1 (0%)	56 58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	138	ASN

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	L	184/184 (100%)	178 (97%)	6 (3%)	45 47
1	M	184/184 (100%)	178 (97%)	6 (3%)	45 47
2	H	186/186 (100%)	184 (99%)	2 (1%)	80 85
2	I	186/186 (100%)	182 (98%)	4 (2%)	60 64
3	P	13/13 (100%)	12 (92%)	1 (8%)	16 12
3	Q	13/13 (100%)	13 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	766/766 (100%)	747 (98%)	19 (2%)	55 59

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	GLU
1	L	91	TYR
1	L	95	LEU
1	L	105	GLU
1	L	108	ARG
1	L	152	ASN
2	H	151	PRO
2	H	221	LYS
1	M	1	GLU
1	M	95	LEU
1	M	105	GLU
1	M	108	ARG
1	M	137	ASN
1	M	143	GLU
2	I	58	ASN
2	I	149	PRO
2	I	151	PRO
2	I	221	LYS
3	P	683	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	11	GLN
1	L	31	ASN
1	L	42	GLN
1	L	100	GLN
1	L	137	ASN
1	L	152	ASN
1	L	210	ASN
2	H	6	GLN
2	H	211	ASN
2	H	216	ASN
1	M	11	GLN
1	M	31	ASN
1	M	37	GLN

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Mol	Chain	Res	Type
1	M	42	GLN
1	M	137	ASN
1	M	138	ASN
1	M	147	GLN
1	M	160	GLN
1	M	198	HIS
1	M	210	ASN
2	I	1	GLN
2	I	3	GLN
2	I	6	GLN
2	I	58	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

2 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	$\#\|Z\| > 2$
3	ORQ	P	677	3	9,10,11	0.51	0	9,11,13	1.43	1 (11%)
3	ORQ	Q	677	3	9,10,11	0.47	0	9,11,13	1.54	2 (22%)

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	ORQ	P	677	3	-	2/7/9/11	0/0/0/0
3	ORQ	Q	677	3	-	2/7/9/11	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Q	677	ORQ	CD-NE-C1	2.19	125.93	122.36
3	P	677	ORQ	C2-C1-NE	2.86	120.54	116.19
3	Q	677	ORQ	C2-C1-NE	2.93	120.64	116.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	Q	677	ORQ	C2-C1-NE-CD
3	P	677	ORQ	C2-C1-NE-CD
3	Q	677	ORQ	O1-C1-NE-CD
3	P	677	ORQ	O1-C1-NE-CD

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	677	ORQ	1	0
3	Q	677	ORQ	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	L	214/214 (100%)	0.41	6 (2%) 56 64	16, 35, 51, 60	0
1	M	214/214 (100%)	0.47	15 (7%) 19 26	14, 30, 62, 85	0
2	H	227/227 (100%)	0.64	15 (6%) 22 29	21, 33, 61, 83	0
2	I	227/227 (100%)	0.50	10 (4%) 38 47	18, 30, 51, 82	0
3	P	13/14 (92%)	0.78	2 (15%) 3 4	22, 32, 71, 75	0
3	Q	13/14 (92%)	0.54	1 (7%) 16 22	18, 21, 58, 63	0
All	All	908/910 (99%)	0.51	49 (5%) 29 38	14, 32, 57, 85	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	134	SER	12.5
2	I	133	THR	10.2
2	H	133	THR	9.0
2	I	128	SER	8.4
2	H	100	TRP	8.2
2	H	130	SER	7.7
2	I	135	GLY	7.5
2	I	130	SER	7.1
2	H	27	GLY	6.7
1	M	154	LEU	5.2
2	H	100(B)	TRP	5.2
2	H	129	LYS	4.6
2	H	135	GLY	4.4
1	L	70	ASP	4.3
3	P	684	LYS	4.1
2	H	127	SER	3.9
2	I	129	LYS	3.7
1	M	203	SER	3.7
1	L	212	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
2	I	100	TRP	3.6
1	M	209	PHE	3.4
2	I	127	SER	3.3
2	H	1	GLN	3.2
1	M	151	ASP	3.1
1	M	213	GLU	3.1
1	L	213	GLU	3.0
1	M	204	PRO	3.0
2	H	100(A)	GLY	3.0
2	H	128	SER	3.0
2	H	199	GLY	2.9
1	M	205	VAL	2.9
2	H	134	SER	2.8
1	M	194	CYS	2.7
3	Q	684	LYS	2.5
1	M	150	VAL	2.5
2	H	136	GLY	2.5
2	H	28	SER	2.4
1	L	16	GLY	2.3
2	I	211	ASN	2.3
1	M	111	ALA	2.3
1	M	202	SER	2.2
1	L	20	THR	2.1
1	M	206	THR	2.1
3	P	683	LYS	2.1
1	L	194	CYS	2.1
1	M	190	LYS	2.1
2	I	225	VAL	2.0
1	M	197	THR	2.0
1	M	210	ASN	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
3	ORQ	Q	677	11/12	0.87	0.16	-	22,25,32,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	ORQ	P	677	11/12	0.85	0.17	-	30,34,38,41	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.