Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:43 AM GMT

PDB ID : 2NZ1
Title : Viral Chemokine Binding Protein M3 From Murine Gammaherpesvirus68 In Complex With The CC-Chemokine CCL2/MCP-1
Authors : Alexander-Brett, J.M.; Fremont, D.H.
Deposited on : 2006-11-22
Resolution : 2.50 Å(reported)

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

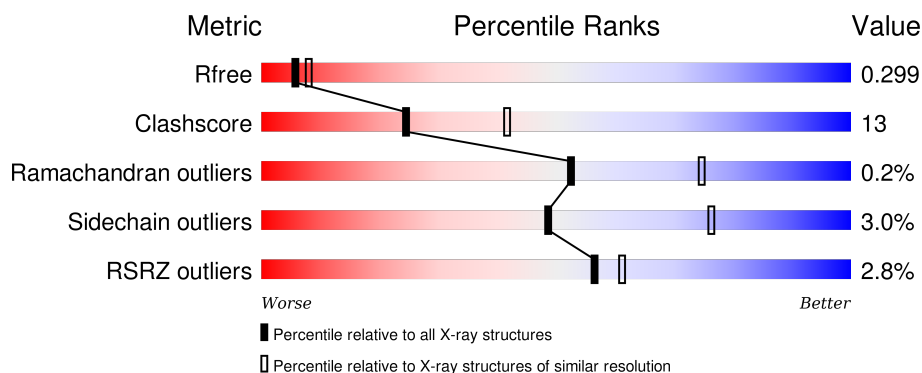|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.50 Å.

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

Metric	Percentile Ranks	Value
Rfree		0.299
Clashscore		13
Ramachandran outliers		0.2%
Sidechain outliers		3.0%
RSRZ outliers		2.8%

Worse ... *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	382	2% — 73% / 24% / •
1	B	382	2% — 70% / 25% / • •
1	X	382	3% — 74% / 21% / • •
2	D	76	5% — 64% / 20% / 16%
2	E	76	3% — 57% / 28% / 16%

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Mol	Chain	Length	Quality of chain
2	Y	76	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10672 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 Hypothetical protein GAMMAHV.M3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	371	Total 2853	C 1798	N 463	O 568	S 24	0	0	0
1	B	371	Total 2853	C 1798	N 463	O 568	S 24	0	0	0
1	X	371	Total 2853	C 1798	N 463	O 568	S 24	0	0	0

- Molecule 2 is a protein called Small inducible cytokine A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	64	Total 517	C 326	N 93	O 94	S 4	0	0	0
2	E	64	Total 517	C 326	N 93	O 94	S 4	0	0	0
2	Y	64	Total 517	C 326	N 93	O 94	S 4	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	64	ILE	MET	ENGINEERED	UNP P13500
E	64	ILE	MET	ENGINEERED	UNP P13500
Y	64	ILE	MET	ENGINEERED	UNP P13500

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	158	Total 158	O 158	0	0
3	B	156	Total 156	O 156	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	36	Total 36	O 36	0	0
3	E	30	Total 30	O 30	0	0
3	X	154	Total 154	O 154	0	0
3	Y	28	Total 28	O 28	0	0

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: Hypothetical protein GAMMAHV.M3

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D103 L104 V105 L108 N114 T115 P116 E117 E118 T119 P120 E121 E122 Y125 A126 Y127 D141 Y150 P159 Y162 V163 D164 V165 L168 A171 V182 W194 I201 S202 E203 E204 S205 L211 C218 S221 V232 C235 T236 A237 E238 M241

Q255 C262 P263 Y266 S271 L279 L284 L287 V296 M297 D302 S303 T304 H305 E306 N307 S312 S313 Y316 H317 C318 P338 L350 V365 S366 L369 E370 G371 Q372 H382

• Molecule 2: Small inducible cytokine A2

Chain D:

5%

64% 20% 16%

GLN PRO ASP ALA ILE ASN ALA P8 C11 N14 F15 T16 K19 R24 V41 I42 F43 V47 A48 K49 E50 D54 P55 K56 W59 V60 K69 Q70 T71 GLN THR PRO LYS THR

• Molecule 2: Small inducible cytokine A2

Chain E:

3%

57% 28% 16%

GLN PRO ASP ALA ILE ASN ALA P8 V9 N14 K19 I20 L25 Y28 R29 R30 I31 E39 A40 V41 I42 F43 V47 E50 I51 D54 P55 K56 Q57 K58 W59 V60 I64 T71 GLN THR PRO LYS THR

• Molecule 2: Small inducible cytokine A2

Chain Y:

5%

62% 22% 16%

GLN PRO ASP ALA ILE ASN ALA P8 T16 L25 Y28 I31 E39 A40 V41 I42 F43 V47 P55 K58 W59 V60 Q61 D62 S63 I64 K69 Q70 T71 GLN THR PRO LYS THR

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	99.24Å 99.24Å 243.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.75 – 2.50 19.75 – 2.30	Depositor EDS
% Data completeness (in resolution range)	93.4 (19.75-2.50) 91.5 (19.75-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	2.76 (at 2.30Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.231 , 0.300 0.231 , 0.299	Depositor DCC
R_{free} test set	2258 reflections (4.94%)	DCC
Wilson B-factor (Å^2)	30.6	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 47.9	EDS
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
L-test for twinning [2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	2 of 61972 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10672	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.50 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.1735e-03.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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 (i)

5.1 Standard geometry (i)

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	0.36	0/2920	0.65	0/3981
1	B	0.36	0/2920	0.67	0/3981
1	X	0.36	0/2920	0.66	1/3981 (0.0%)
2	D	0.35	0/526	0.63	0/708
2	E	0.35	0/526	0.62	0/708
2	Y	0.35	0/526	0.62	0/708
All	All	0.36	0/10338	0.65	1/14067 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	307	ASN	N-CA-C	-5.41	96.41	111.00

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	2853	0	2763	65	0
1	B	2853	0	2763	89	0
1	X	2853	0	2763	75	0
2	D	517	0	531	12	0
2	E	517	0	531	17	0
2	Y	517	0	531	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	158	0	0	8	0
3	B	156	0	0	8	0
3	D	36	0	0	2	0
3	E	30	0	0	0	0
3	X	154	0	0	8	0
3	Y	28	0	0	2	0
All	All	10672	0	9882	257	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 (257) 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:B:131:GLN:HE21	1:B:170:ARG:HH12	1.05	1.01
1:B:81:GLU:O	2:D:24:ARG:HD3	1.65	0.95
1:X:90:ARG:HB3	1:X:90:ARG:HH11	1.34	0.91
1:X:201:ILE:HD13	1:X:205:SER:HB2	1.53	0.89
1:X:99:THR:HG21	1:X:313:SER:O	1.72	0.88
1:B:87:ILE:HG21	1:B:200:ALA:HB2	1.57	0.84
2:E:54:ASP:HB3	2:E:57:GLN:HG3	1.57	0.84
1:A:82:LEU:HD21	2:E:51:ILE:HD11	1.60	0.82
1:X:171:ALA:HB2	1:X:182:VAL:HG21	1.62	0.81
1:B:131:GLN:NE2	1:B:170:ARG:HH12	1.78	0.80
1:A:99:THR:HG22	1:A:101:VAL:H	1.47	0.78
1:B:284:LEU:HD21	1:B:369:LEU:HD13	1.66	0.76
1:X:284:LEU:HD21	1:X:369:LEU:HD13	1.69	0.73
1:A:233:ASP:O	1:A:243:LYS:HD2	1.87	0.73
1:B:99:THR:HG22	1:B:101:VAL:H	1.52	0.73
1:X:103:ASP:HB3	3:X:437:HOH:O	1.90	0.71
2:D:41:VAL:HG23	2:D:55:PRO:HG3	1.72	0.71
1:X:203:GLU:HG3	3:X:409:HOH:O	1.92	0.69
1:X:236:THR:OG1	1:X:238:GLU:HG2	1.93	0.69
1:B:30:ASP:HB2	3:B:427:HOH:O	1.91	0.69
1:B:114:ASN:ND2	1:B:179:GLY:HA3	2.08	0.68
1:B:41:GLU:OE2	1:B:46:GLU:HG2	1.92	0.68
1:A:131:GLN:CD	1:A:170:ARG:HH22	1.95	0.68
1:X:90:ARG:HB3	1:X:90:ARG:NH1	2.08	0.68
1:B:127:TYR:O	3:B:519:HOH:O	2.11	0.67
1:X:211:LEU:HD23	1:X:372:GLN:HG2	1.76	0.67
1:A:100:PRO:HB3	1:B:100:PRO:HA	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:THR:HG22	1:B:170:ARG:HG3	1.78	0.66
1:A:74:VAL:HG21	1:A:88:THR:O	1.95	0.66
1:X:171:ALA:CB	1:X:182:VAL:HG21	2.26	0.65
1:X:51:LEU:HB3	1:X:55:LEU:HD22	1.78	0.65
1:B:236:THR:OG1	1:B:238:GLU:HG2	1.97	0.64
2:Y:31:ILE:CD1	2:Y:40:ALA:HB3	2.27	0.64
1:B:37:LEU:HD21	1:B:108:LEU:HD22	1.80	0.64
2:Y:31:ILE:HD12	2:Y:40:ALA:HB3	1.79	0.64
1:A:50:ILE:O	1:A:54:VAL:HG23	1.97	0.64
1:B:60:HIS:HB3	1:B:63:GLN:HE21	1.62	0.64
1:B:99:THR:HG21	1:B:313:SER:O	1.98	0.63
1:A:30:ASP:HB2	3:A:481:HOH:O	1.98	0.63
1:A:115:THR:HG23	3:A:500:HOH:O	1.99	0.62
2:Y:70:GLN:HG3	2:Y:71:THR:H	1.64	0.61
1:X:94:PRO:HD3	1:X:194:TRP:CE2	2.36	0.60
2:Y:39:GLU:HG2	2:Y:55:PRO:HG2	1.82	0.60
1:X:287:LEU:HD11	1:X:350:LEU:HB3	1.82	0.60
1:A:82:LEU:HD21	2:E:51:ILE:CD1	2.31	0.60
1:B:171:ALA:HB2	1:B:182:VAL:HG21	1.84	0.60
1:A:203:GLU:HG3	3:A:400:HOH:O	2.00	0.60
1:B:171:ALA:CB	1:B:182:VAL:HG21	2.32	0.60
2:Y:58:LYS:HG2	2:Y:62:ASP:OD2	2.02	0.60
1:X:74:VAL:HG21	1:X:88:THR:O	2.02	0.59
1:A:100:PRO:HG2	1:B:161:SER:OG	2.03	0.59
1:B:278:HIS:CD2	1:B:353:ARG:HD3	2.37	0.59
1:X:350:LEU:C	1:X:350:LEU:HD12	2.23	0.59
1:B:114:ASN:HD21	1:X:117:GLU:HB3	1.68	0.59
2:E:60:VAL:O	2:E:64:ILE:HG13	2.04	0.58
1:X:104:LEU:HD12	1:X:159:PRO:HA	1.85	0.58
2:E:20:ILE:HD13	2:E:51:ILE:HD12	1.86	0.58
1:X:201:ILE:CD1	1:X:205:SER:HB2	2.30	0.58
1:X:115:THR:HG22	1:X:150:TYR:CD2	2.39	0.57
1:A:131:GLN:OE1	1:A:170:ARG:NH2	2.37	0.57
2:Y:47:VAL:O	2:Y:47:VAL:HG12	2.04	0.57
1:X:90:ARG:HG2	1:X:168:LEU:CD1	2.35	0.57
1:X:99:THR:HG23	1:X:101:VAL:H	1.69	0.57
2:E:28:TYR:CZ	2:E:64:ILE:HG23	2.40	0.57
2:Y:28:TYR:CD1	2:Y:64:ILE:HD12	2.40	0.56
1:B:74:VAL:O	1:B:200:ALA:HA	2.05	0.56
1:B:202:SER:HB3	1:B:204:GLU:HG2	1.88	0.56
1:B:203:GLU:HG3	3:B:431:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:LEU:C	1:B:350:LEU:HD12	2.26	0.56
1:A:60:HIS:HB3	1:A:63:GLN:OE1	2.05	0.56
1:B:345:GLN:HE22	1:B:351:GLN:NE2	2.04	0.56
1:X:297:MET:O	1:X:365:VAL:HA	2.05	0.56
1:X:87:ILE:HD11	1:X:182:VAL:HG23	1.88	0.56
1:X:72:MET:HB3	3:X:443:HOH:O	2.05	0.55
1:A:94:PRO:HD3	1:A:194:TRP:CE2	2.41	0.55
1:X:235:CYS:HB3	1:X:241:MET:HE3	1.89	0.55
2:E:41:VAL:HG23	2:E:55:PRO:HG3	1.88	0.55
2:E:47:VAL:O	2:E:47:VAL:HG12	2.06	0.54
1:B:179:GLY:CA	1:X:117:GLU:HB3	2.37	0.54
1:B:335:GLU:HG2	1:B:336:GLN:N	2.22	0.54
1:B:37:LEU:CD2	1:B:108:LEU:HD22	2.37	0.54
1:B:302:ASP:OD2	1:B:304:THR:HG23	2.08	0.54
1:X:86:ILE:N	1:X:86:ILE:HD12	2.23	0.54
1:B:51:LEU:HB3	1:B:55:LEU:HD22	1.90	0.54
1:A:343:GLU:HB2	3:A:411:HOH:O	2.08	0.54
1:B:345:GLN:H	1:B:345:GLN:CD	2.12	0.53
1:B:72:MET:HB3	3:B:430:HOH:O	2.08	0.53
2:E:25:LEU:HD22	2:E:43:PHE:HB3	1.89	0.53
1:A:272:PRO:HA	2:D:11:CYS:O	2.09	0.53
1:X:87:ILE:HG13	1:X:87:ILE:O	2.08	0.53
1:B:287:LEU:HD11	1:B:350:LEU:HB3	1.90	0.53
1:B:131:GLN:NE2	1:B:170:ARG:NH1	2.55	0.52
1:B:104:LEU:N	1:B:104:LEU:HD12	2.24	0.52
1:A:307:ASN:ND2	1:B:42:THR:HB	2.24	0.52
1:B:94:PRO:HD3	1:B:194:TRP:CE2	2.44	0.52
1:B:112:GLU:HB3	1:B:151:MET:HG3	1.92	0.52
1:B:131:GLN:HE21	1:B:170:ARG:NH1	1.89	0.51
2:D:47:VAL:HG12	2:D:47:VAL:O	2.11	0.51
1:B:185:MET:HG2	1:B:195:CYS:SG	2.50	0.51
1:X:221:SER:HA	3:X:469:HOH:O	2.11	0.51
1:B:139:LEU:HD12	1:B:154:TRP:HB3	1.92	0.51
1:A:99:THR:HG21	1:A:313:SER:O	2.11	0.51
1:B:85:GLU:HG3	1:B:176:GLN:HG3	1.92	0.51
1:X:75:PRO:HG3	1:X:201:ILE:HD11	1.93	0.51
1:X:41:GLU:OE2	1:X:46:GLU:HG2	2.10	0.51
1:X:22:ASP:HB3	1:X:25:GLN:HG3	1.93	0.50
1:X:99:THR:CG2	1:X:101:VAL:H	2.25	0.50
2:Y:28:TYR:CE1	2:Y:64:ILE:HD12	2.47	0.50
1:B:27:LYS:HB3	1:B:27:LYS:NZ	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:PRO:HD2	1:B:162:TYR:HD2	1.75	0.50
1:A:181:LYS:HD3	3:A:533:HOH:O	2.12	0.50
1:X:232:VAL:HG23	3:X:393:HOH:O	2.12	0.50
1:B:87:ILE:HG21	1:B:200:ALA:CB	2.37	0.50
2:Y:70:GLN:HG3	2:Y:71:THR:N	2.27	0.50
1:A:71:LYS:O	1:A:210:SER:HB3	2.12	0.50
1:X:235:CYS:HB3	1:X:241:MET:CE	2.42	0.49
1:X:318:CYS:SG	1:X:338:PRO:HD2	2.51	0.49
1:B:88:THR:CG2	1:B:170:ARG:HG3	2.43	0.49
1:B:169:THR:HB	1:B:198:LEU:HD11	1.95	0.49
1:A:246:LEU:HA	1:A:258:LYS:HG2	1.95	0.49
1:A:69:LYS:HE3	1:A:197:GLU:OE1	2.13	0.49
1:A:99:THR:HG23	1:A:100:PRO:HD2	1.94	0.49
1:A:98:GLY:HA2	1:A:315:LEU:HD23	1.95	0.49
1:X:255:GLN:HB3	1:X:284:LEU:HD11	1.95	0.48
1:B:54:VAL:HG12	1:B:55:LEU:HD13	1.95	0.48
1:A:247:LEU:HD11	1:A:259:MET:HB3	1.95	0.48
1:B:179:GLY:HA3	1:X:117:GLU:HB3	1.94	0.48
2:E:28:TYR:HA	2:E:42:ILE:O	2.13	0.48
2:E:31:ILE:HD11	2:E:42:ILE:HD11	1.96	0.48
1:A:269:SER:HB3	1:A:273:LEU:HD11	1.96	0.48
1:A:131:GLN:HA	1:A:136:THR:HA	1.95	0.48
1:A:244:MET:SD	1:A:260:ASN:HB2	2.53	0.48
1:B:296:VAL:HG21	1:B:341:LEU:HD21	1.95	0.48
1:A:284:LEU:HB3	1:A:350:LEU:HG	1.95	0.48
1:A:255:GLN:HB3	1:A:284:LEU:HD11	1.96	0.48
2:Y:60:VAL:O	2:Y:64:ILE:HG12	2.13	0.48
1:B:76:TRP:CE3	1:B:85:GLU:HB3	2.49	0.48
1:X:296:VAL:HA	1:X:366:SER:O	2.14	0.48
1:A:296:VAL:HA	1:A:366:SER:O	2.14	0.47
1:A:112:GLU:O	1:A:180:ALA:HA	2.13	0.47
1:B:74:VAL:HG21	1:B:88:THR:O	2.14	0.47
2:D:16:THR:HG23	2:D:16:THR:O	2.14	0.47
1:A:115:THR:HG22	1:A:150:TYR:CD2	2.50	0.47
1:X:302:ASP:HB2	1:X:316:TYR:CE1	2.50	0.47
2:D:19:LYS:HG3	2:D:59:TRP:CE3	2.49	0.47
1:B:103:ASP:HB3	3:B:531:HOH:O	2.14	0.47
1:X:218:CYS:C	3:X:469:HOH:O	2.53	0.47
1:A:36:CYS:O	1:A:106:ARG:HG2	2.15	0.47
1:X:84:GLN:HB3	1:X:86:ILE:HD11	1.95	0.47
1:B:246:LEU:HA	1:B:258:LYS:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:75:PRO:HA	1:X:201:ILE:O	2.15	0.46
1:X:211:LEU:HB3	1:X:371:GLY:O	2.15	0.46
2:Y:61:GLN:HB3	3:Y:103:HOH:O	2.14	0.46
1:A:139:LEU:HB3	1:A:154:TRP:CG	2.50	0.46
1:A:161:SER:OG	1:B:100:PRO:HG2	2.15	0.46
1:B:90:ARG:HG2	1:B:168:LEU:HD12	1.96	0.46
1:B:99:THR:HG22	1:B:101:VAL:N	2.27	0.46
1:B:365:VAL:HG22	1:B:378:TYR:HE2	1.81	0.46
1:X:54:VAL:HG11	1:X:61:GLU:OE2	2.16	0.46
1:B:335:GLU:HG2	1:B:336:GLN:H	1.80	0.46
1:X:302:ASP:HB2	1:X:316:TYR:HE1	1.81	0.46
1:X:86:ILE:HG23	1:X:171:ALA:O	2.16	0.45
1:X:76:TRP:HB2	1:X:203:GLU:HG2	1.99	0.45
1:B:335:GLU:HG2	1:B:336:GLN:HG2	1.98	0.45
2:E:20:ILE:CD1	2:E:51:ILE:HD12	2.46	0.45
1:A:269:SER:O	2:D:14:ASN:HB2	2.16	0.45
1:X:305:HIS:CE1	1:X:306:GLU:O	2.69	0.45
1:X:266:TYR:CD2	1:X:279:LEU:HD11	2.51	0.45
1:A:105:VAL:HG11	1:A:163:VAL:HG21	1.99	0.45
1:X:202:SER:HB2	1:X:205:SER:OG	2.16	0.45
1:X:241:MET:HE3	1:X:262:CYS:HB3	1.98	0.45
1:X:116:PRO:HG2	1:X:120:PRO:HD3	1.99	0.44
1:B:262:CYS:N	1:B:263:PRO:CD	2.79	0.44
1:A:311:PRO:HD2	3:B:451:HOH:O	2.16	0.44
1:B:99:THR:HG23	1:B:100:PRO:HD2	1.99	0.44
1:A:202:SER:O	1:A:205:SER:HB2	2.16	0.44
1:X:116:PRO:HD2	1:X:150:TYR:CZ	2.52	0.44
2:D:43:PHE:CZ	2:D:60:VAL:HG13	2.53	0.44
1:B:31:GLU:HB3	1:B:50:ILE:HD13	2.00	0.44
1:B:117:GLU:HG2	1:X:114:ASN:OD1	2.18	0.43
1:A:100:PRO:HA	1:B:100:PRO:HB3	2.00	0.43
1:A:131:GLN:NE2	1:A:170:ARG:HH22	2.16	0.43
1:B:82:LEU:HD13	3:D:92:HOH:O	2.17	0.43
1:B:46:GLU:O	1:B:50:ILE:HG13	2.18	0.43
1:A:323:THR:O	1:A:329:TRP:HA	2.18	0.43
1:B:139:LEU:N	1:B:139:LEU:HD22	2.32	0.43
1:A:117:GLU:HG3	1:A:118:GLU:HG2	2.00	0.43
1:B:43:GLU:HA	1:B:43:GLU:OE1	2.19	0.43
2:Y:71:THR:HG21	3:Y:89:HOH:O	2.18	0.43
1:A:159:PRO:HD2	1:A:162:TYR:HD2	1.84	0.43
1:X:75:PRO:HA	1:X:201:ILE:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:164:ASP:OD1	1:X:165:VAL:N	2.45	0.43
1:A:96:VAL:HG23	3:A:441:HOH:O	2.18	0.43
1:X:262:CYS:N	1:X:263:PRO:CD	2.82	0.43
1:X:30:ASP:OD1	1:X:31:GLU:HG3	2.19	0.43
1:B:164:ASP:OD1	1:B:165:VAL:N	2.50	0.43
1:X:201:ILE:HD12	1:X:201:ILE:C	2.39	0.42
1:X:305:HIS:ND1	1:X:306:GLU:O	2.52	0.42
1:X:105:VAL:HG13	1:X:105:VAL:O	2.20	0.42
1:X:32:ILE:HG21	1:X:65:LEU:HD11	2.01	0.42
1:B:244:MET:SD	1:B:260:ASN:HB2	2.60	0.42
1:B:345:GLN:CD	1:B:345:GLN:N	2.72	0.42
1:A:171:ALA:HB2	1:A:182:VAL:HG21	2.02	0.42
1:B:125:TYR:HB3	1:B:174:LEU:HG	2.02	0.42
1:X:159:PRO:HD2	1:X:162:TYR:HD2	1.85	0.42
1:B:94:PRO:HD3	1:B:194:TRP:CZ2	2.54	0.42
1:B:51:LEU:HB3	1:B:55:LEU:CD2	2.48	0.42
2:E:43:PHE:O	2:E:50:GLU:HA	2.20	0.42
1:B:257:ALA:HB2	1:B:284:LEU:HD13	2.00	0.42
1:A:290:LEU:HD12	3:A:432:HOH:O	2.20	0.42
1:B:147:THR:HG22	1:B:152:THR:HG23	2.02	0.42
1:A:211:LEU:HD23	1:A:372:GLN:HG2	2.01	0.42
1:X:84:GLN:CB	1:X:86:ILE:HD11	2.50	0.42
1:X:93:PHE:HB3	3:X:448:HOH:O	2.19	0.42
1:B:323:THR:HG22	1:B:324:SER:N	2.35	0.42
1:B:313:SER:HB3	3:B:516:HOH:O	2.20	0.42
1:B:36:CYS:O	1:B:106:ARG:HG2	2.20	0.42
1:A:148:SER:OG	1:A:151:MET:HB3	2.20	0.42
1:A:177:TRP:HA	1:A:178:PRO:HD3	1.87	0.42
1:A:185:MET:HG2	1:A:195:CYS:SG	2.60	0.42
1:B:108:LEU:HA	1:B:108:LEU:HD12	1.94	0.41
2:Y:41:VAL:HG23	2:Y:55:PRO:HG3	2.02	0.41
1:X:125:TYR:OH	1:X:127:TYR:HB2	2.20	0.41
1:X:369:LEU:HD23	1:X:369:LEU:N	2.36	0.41
2:D:43:PHE:O	2:D:50:GLU:HA	2.20	0.41
1:B:323:THR:O	1:B:329:TRP:HA	2.20	0.41
1:A:132:THR:HG22	3:A:455:HOH:O	2.20	0.41
1:A:266:TYR:CD2	1:A:279:LEU:HD11	2.56	0.41
1:B:179:GLY:HA2	1:X:117:GLU:HB3	2.02	0.41
1:X:116:PRO:HD2	1:X:150:TYR:CE1	2.55	0.41
1:X:221:SER:N	3:X:469:HOH:O	2.53	0.41
1:A:91:LEU:HD13	1:A:196:GLY:HA3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:THR:HB	1:A:170:ARG:HG3	2.03	0.41
1:B:164:ASP:O	1:B:165:VAL:C	2.59	0.41
2:E:19:LYS:HG3	2:E:59:TRP:CE3	2.56	0.41
1:B:361:ASN:ND2	3:B:442:HOH:O	2.52	0.41
1:B:76:TRP:HB2	1:B:203:GLU:HG2	2.03	0.41
1:A:284:LEU:HD21	1:A:369:LEU:HD13	2.02	0.41
1:A:110:VAL:O	1:A:182:VAL:HA	2.21	0.41
2:D:70:GLN:O	2:D:70:GLN:HG3	2.20	0.41
2:D:54:ASP:HA	2:D:55:PRO:HD3	1.90	0.41
1:A:279:LEU:HG	1:A:356:PRO:HG3	2.03	0.41
1:X:303:SER:O	1:X:304:THR:C	2.59	0.41
1:B:74:VAL:HA	1:B:75:PRO:HD3	1.79	0.40
2:E:29:ARG:CZ	2:E:42:ILE:HD12	2.50	0.40
2:E:39:GLU:HG2	2:E:55:PRO:HG2	2.02	0.40
1:A:139:LEU:HD12	1:A:154:TRP:HB3	2.01	0.40
1:A:345:GLN:NE2	1:A:345:GLN:HA	2.36	0.40
1:A:82:LEU:HB2	1:A:84:GLN:HG3	2.03	0.40
1:B:269:SER:O	2:E:14:ASN:HB2	2.21	0.40
2:Y:25:LEU:HD22	2:Y:43:PHE:HB3	2.02	0.40
2:Y:16:THR:O	2:Y:16:THR:HG23	2.21	0.40
1:X:201:ILE:HD12	1:X:201:ILE:O	2.21	0.40
1:X:74:VAL:HA	1:X:75:PRO:HD3	1.87	0.40
1:A:88:THR:HA	1:A:169:THR:O	2.22	0.40
1:A:350:LEU:HD12	1:A:350:LEU:C	2.42	0.40
2:D:56:LYS:NZ	3:D:83:HOH:O	2.54	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	369/382 (97%)	348 (94%)	20 (5%)	1 (0%)	46	68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	369/382 (97%)	346 (94%)	22 (6%)	1 (0%)	46	68
1	X	369/382 (97%)	341 (92%)	28 (8%)	0	100	100
2	D	62/76 (82%)	59 (95%)	3 (5%)	0	100	100
2	E	62/76 (82%)	59 (95%)	2 (3%)	1 (2%)	12	21
2	Y	62/76 (82%)	60 (97%)	2 (3%)	0	100	100
All	All	1293/1374 (94%)	1213 (94%)	77 (6%)	3 (0%)	52	75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	LYS
2	E	9	VAL
1	B	311	PRO

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	327/335 (98%)	319 (98%)	8 (2%)	57	82
1	B	327/335 (98%)	314 (96%)	13 (4%)	38	64
1	X	327/335 (98%)	313 (96%)	14 (4%)	35	61
2	D	60/70 (86%)	60 (100%)	0	100	100
2	E	60/70 (86%)	60 (100%)	0	100	100
2	Y	60/70 (86%)	60 (100%)	0	100	100
All	All	1161/1215 (96%)	1126 (97%)	35 (3%)	48	76

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	33	GLN
1	A	88	THR

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Mol	Chain	Res	Type
1	A	104	LEU
1	A	122	GLU
1	A	141	ASP
1	A	142	ASP
1	A	271	SER
1	B	33	GLN
1	B	55	LEU
1	B	81	GLU
1	B	99	THR
1	B	108	LEU
1	B	122	GLU
1	B	204	GLU
1	B	271	SER
1	B	306	GLU
1	B	335	GLU
1	B	350	LEU
1	B	365	VAL
1	B	376	LEU
1	X	25	GLN
1	X	30	ASP
1	X	33	GLN
1	X	81	GLU
1	X	90	ARG
1	X	99	THR
1	X	104	LEU
1	X	108	LEU
1	X	122	GLU
1	X	141	ASP
1	X	238	GLU
1	X	271	SER
1	X	305	HIS
1	X	350	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	208	GLN
1	A	305	HIS
1	A	345	GLN
1	B	33	GLN
1	B	58	ASN

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Mol	Chain	Res	Type
1	B	60	HIS
1	B	63	GLN
1	B	114	ASN
1	B	131	GLN
1	B	208	GLN
1	B	351	GLN
1	B	361	ASN
2	D	17	ASN
2	D	23	GLN
1	X	33	GLN
1	X	63	GLN
1	X	345	GLN
2	Y	23	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	371/382 (97%)	-0.15	7 (1%)	70	73	15, 32, 68, 95	0
1	B	371/382 (97%)	-0.20	9 (2%)	62	66	16, 33, 70, 95	0
1	X	371/382 (97%)	-0.17	10 (2%)	58	62	15, 33, 71, 98	0
2	D	64/76 (84%)	-0.08	4 (6%)	23	26	20, 38, 56, 85	0
2	E	64/76 (84%)	-0.17	2 (3%)	52	57	20, 37, 63, 91	0
2	Y	64/76 (84%)	-0.20	4 (6%)	23	26	22, 36, 59, 85	0
All	All	1305/1374 (94%)	-0.17	36 (2%)	56	61	15, 33, 70, 98	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	382	HIS	5.9
1	X	382	HIS	5.6
1	X	119	THR	5.4
1	B	382	HIS	4.3
1	B	79	VAL	4.2
1	X	121	GLU	4.1
2	Y	71	THR	4.0
1	A	12	HIS	3.8
1	B	12	HIS	3.6
2	E	71	THR	3.4
1	A	121	GLU	3.3
1	B	335	GLU	3.2
1	A	117	GLU	3.1
2	D	69	LYS	3.1
1	X	305	HIS	3.1
1	B	24	SER	2.9
1	A	119	THR	2.9
1	B	305	HIS	2.9
1	X	12	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	305	HIS	2.8
2	E	8	PRO	2.6
1	X	304	THR	2.4
1	X	303	SER	2.4
1	A	312	SER	2.4
2	Y	70	GLN	2.4
1	X	312	SER	2.3
2	Y	69	LYS	2.2
1	X	79	VAL	2.1
2	D	8	PRO	2.1
2	D	71	THR	2.1
2	D	48	ALA	2.1
1	B	121	GLU	2.0
1	B	174	LEU	2.0
1	B	85	GLU	2.0
1	X	118	GLU	2.0
2	Y	8	PRO	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.