Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:02 PM GMT

PDB ID	:	3VVA
Title	:	Crystal structure of cyanide-insensitive alternative oxidase from Trypanosoma brucei with ascofuranone derivative
Authors	:	Shiba, T.; Kido, Y.; Sakamoto, K.; Inaoka, D.K.; Tsuge, C.; Tatsumi, R.; Balogun, E.O.; Nara, T.; Aoki, T.; Honma, T.; Tanaka, A.; Inoue, M.; Matsuoka, S.; Saimoto, H.; Moore, A.L.; Harada, S.; Kita, K.
Deposited on	:	2012-07-17
Resolution	:	2.59 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:

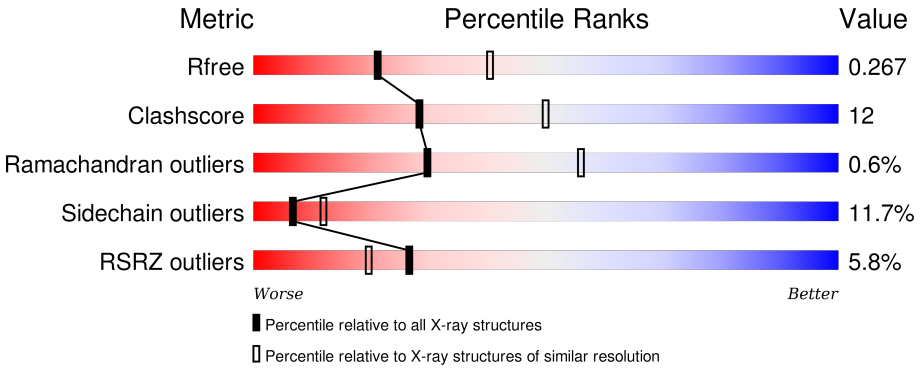
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.59 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	329	3% 48% 28% 5% 19%
1	B	329	2% 57% 20% • 19%
1	C	329	6% 55% 21% 5% 19%
1	D	329	8% 58% 19% • 19%

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FE	B	502	-	-	-	X
2	FE	D	502	-	-	-	X
4	CHW	D	504	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8885 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.

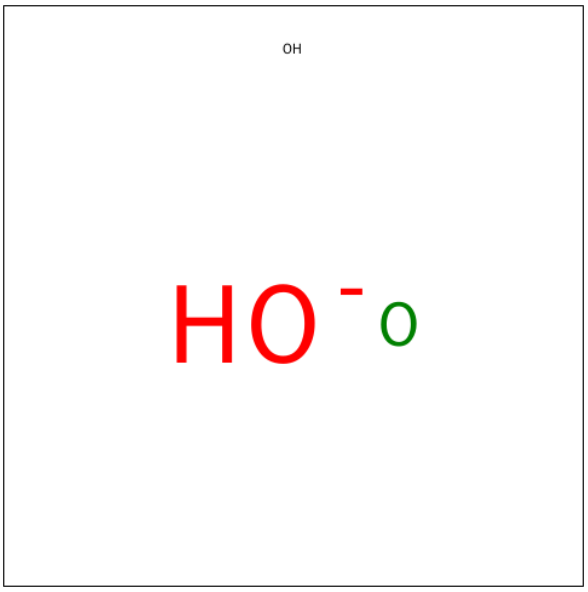
- Molecule 1 is a protein called Alternative oxidase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	0	0	0
			2160	1384	383	383	10			
1	B	265	Total	C	N	O	S	0	0	0
			2155	1381	383	381	10			
1	C	266	Total	C	N	O	S	0	1	0
			2171	1392	386	383	10			
1	D	266	Total	C	N	O	S	0	0	0
			2160	1384	383	383	10			

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

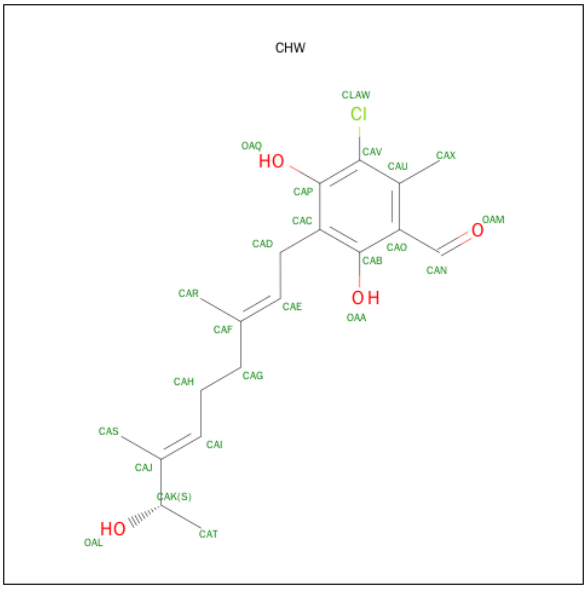
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Fe	0	0
			2	2		
2	A	2	Total	Fe	0	0
			2	2		
2	D	2	Total	Fe	0	0
			2	2		
2	C	2	Total	Fe	0	0
			2	2		

- Molecule 3 is HYDROXIDE ION (three-letter code: OH) (formula: HO).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O 1 1	0	0
3	B	1	Total O 1 1	0	0
3	C	1	Total O 1 1	0	0
3	D	1	Total O 1 1	0	0

- Molecule 4 is 3-CHLORO-4,6-DIHYDROXY-5-[(2E,6E,8S)-8-HYDROXY-3,7-DIMETHYLNONA-2,6-DIEN-1-YL]-2-METHYLBENZALDEHYDE (three-letter code: CHW) (formula: $C_{19}H_{25}ClO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	Cl	O	0	0
			24	19	1	4		
4	B	1	Total	C	Cl	O	0	0
			24	19	1	4		
4	C	1	Total	C	Cl	O	0	0
			24	19	1	4		
4	D	1	Total	C	Cl	O	0	0
			24	19	1	4		

- Molecule 5 is water.

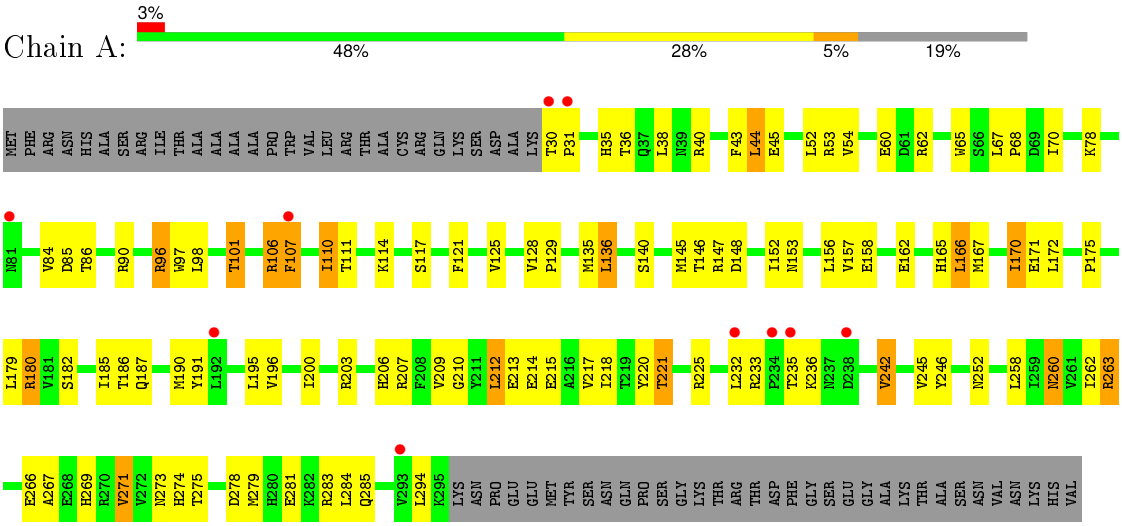
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	35	Total	O	0	0
			35	35		
5	B	39	Total	O	0	0
			39	39		
5	C	21	Total	O	0	0
			21	21		
5	D	36	Total	O	0	0
			36	36		

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.

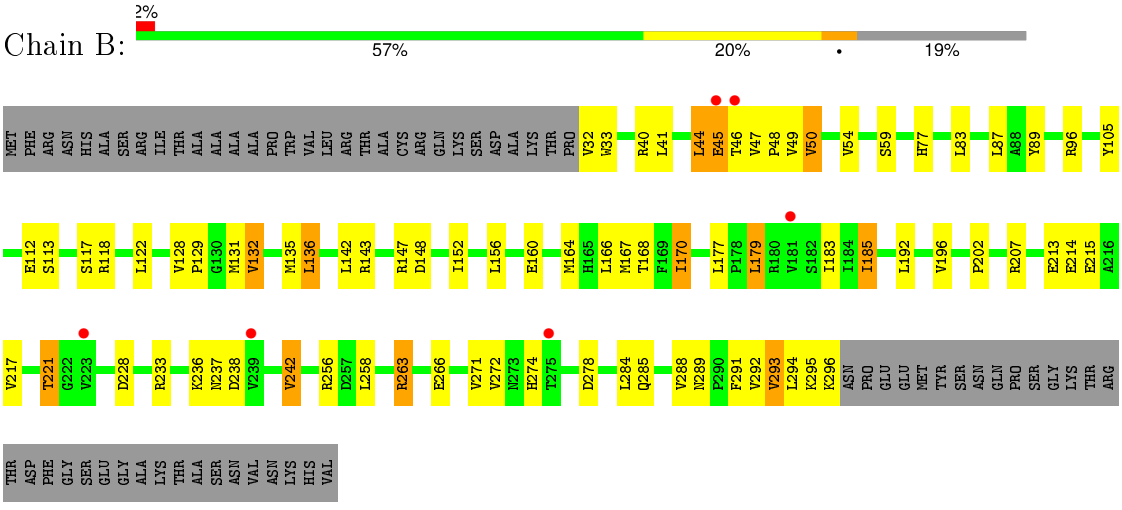
- Molecule 1: Alternative oxidase, mitochondrial

Chain A:



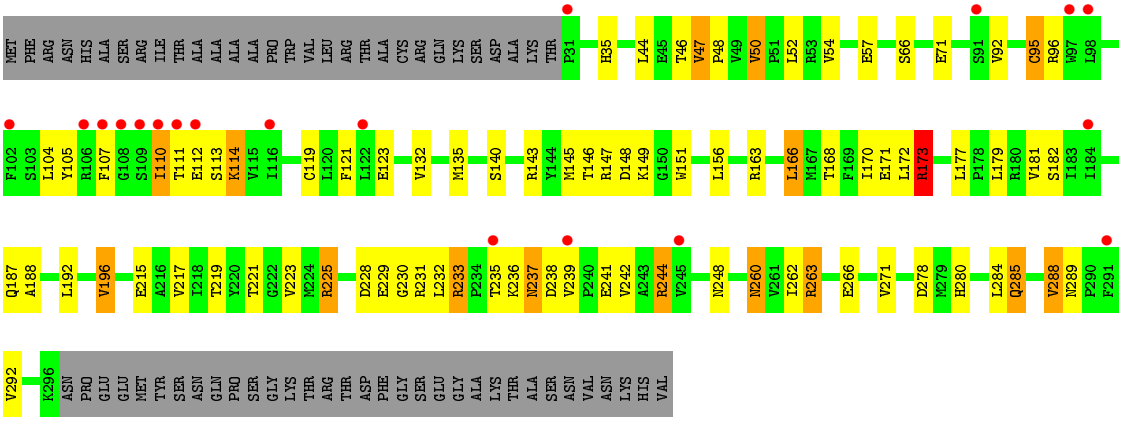
- Molecule 1: Alternative oxidase, mitochondrial

Chain B:



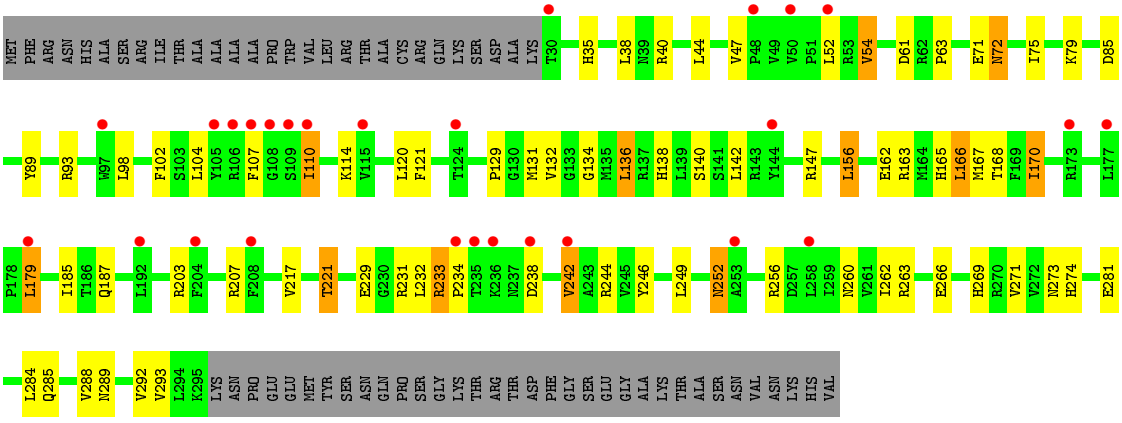
- Molecule 1: Alternative oxidase, mitochondrial

Chain C:



• Molecule 1: Alternative oxidase, mitochondrial

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	152.31Å 219.68Å 63.48Å 90.00° 114.89° 90.00°	Depositor
Resolution (Å)	39.81 – 2.59 39.81 – 2.59	Depositor EDS
% Data completeness (in resolution range)	92.2 (39.81-2.59) 97.1 (39.81-2.59)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.214 , 0.256 0.222 , 0.267	Depositor DCC
R_{free} test set	2885 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	44.8	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 23.0	EDS
Estimated twinning fraction	0.448 for H, K, L 0.552 for H+4/2L, -K, -L 0.136 for -h-2*l,-k,l	Xtriage
Reported twinning fraction	0.448 for H, K, L 0.552 for H+4/2L, -K, -L	Depositor
L-test for twinning[2]	$< \|L\| > = 0.54$, $< L^2 > = 0.38$	Xtriage
Outliers	1 of 56974 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	8885	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.86% 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: CHW, FE, OH

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	0.46	0/2210	0.69	0/3004
1	B	0.42	0/2204	0.64	0/2993
1	C	0.40	0/2221	0.60	0/3015
1	D	0.39	0/2210	0.61	0/3004
All	All	0.42	0/8845	0.64	0/12016

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	2160	0	2189	77	0
1	B	2155	0	2188	60	0
1	C	2171	0	2208	53	0
1	D	2160	0	2189	48	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	1	0
4	A	24	0	23	3	0
4	B	24	0	23	3	0
4	C	24	0	24	3	0
4	D	24	0	23	0	0
5	A	35	0	0	0	0
5	B	39	0	0	1	0
5	C	21	0	0	0	0
5	D	36	0	0	1	0
All	All	8885	0	8867	204	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 12.

All (204) 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:217:VAL:O	1:B:221:THR:HG23	1.58	1.02
1:C:192:LEU:O	1:C:196:VAL:HG12	1.74	0.87
1:A:135:MET:HE1	1:A:136:LEU:HD13	1.59	0.84
1:C:221:THR:HG22	1:C:263:ARG:NE	1.94	0.82
1:C:121:PHE:HE1	4:C:504:CHW:HAT	1.48	0.79
1:C:221:THR:HG22	1:C:263:ARG:HE	1.48	0.78
1:A:40:ARG:O	1:B:271:VAL:HG12	1.84	0.77
1:C:46:THR:O	1:C:50:VAL:HG12	1.85	0.76
1:A:30:THR:N	1:A:31:PRO:HD2	2.02	0.75
1:C:217:VAL:O	1:C:221:THR:HG23	1.88	0.73
1:D:207:ARG:HH11	1:D:274:HIS:HD2	1.34	0.73
1:A:135:MET:HG3	1:B:135:MET:CE	2.19	0.72
1:D:289:ASN:O	1:D:292:VAL:HG22	1.90	0.71
1:A:283:ARG:HA	1:A:285:GLN:NE2	2.04	0.71
1:C:215:GLU:HB3	4:C:504:CHW:HAD	1.73	0.71
1:B:202:PRO:HD2	5:B:625:HOH:O	1.90	0.70
1:C:111:THR:H	1:C:114:LYS:HE3	1.58	0.68
1:B:207:ARG:HH11	1:B:274:HIS:HD2	1.40	0.67
1:A:110:ILE:HG12	1:A:232:LEU:HD22	1.76	0.67
1:A:172:LEU:HD22	1:A:236:LYS:HD2	1.76	0.67
1:D:44:LEU:O	1:D:47:VAL:HG12	1.94	0.66
1:A:148:ASP:OD1	1:A:152:ILE:HG13	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:GLU:HA	1:C:244:ARG:HB2	1.78	0.65
1:A:167:MET:CE	1:B:147:ARG:HD3	2.26	0.65
1:A:44:LEU:HG	1:B:278:ASP:HB3	1.80	0.63
1:A:167:MET:HE2	1:B:147:ARG:HH11	1.64	0.63
1:D:110:ILE:HA	1:D:114:LYS:HD3	1.80	0.62
1:D:75:ILE:HD11	1:D:221:THR:HG21	1.81	0.62
1:A:175:PRO:HG2	1:A:180:ARG:HD3	1.81	0.62
1:C:172:LEU:O	1:C:173:ARG:HB2	1.98	0.62
1:A:167:MET:HE2	1:B:147:ARG:HD3	1.83	0.61
1:C:143:ARG:HH11	1:D:187:GLN:NE2	1.99	0.61
1:D:217:VAL:O	1:D:221:THR:HG22	2.00	0.60
1:A:207:ARG:HH11	1:A:274:HIS:HD2	1.49	0.60
1:D:269:HIS:O	1:D:273:ASN:HB2	2.01	0.60
1:B:217:VAL:O	1:B:221:THR:CG2	2.45	0.60
1:A:86:THR:HG22	1:A:90:ARG:HD2	1.84	0.60
1:B:293:VAL:C	1:B:295:LYS:H	2.05	0.59
1:C:235:THR:C	1:C:237:ASN:H	2.06	0.59
1:B:45:GLU:H	1:B:45:GLU:CD	2.06	0.59
1:B:221:THR:HB	1:B:263:ARG:HH21	1.68	0.59
1:A:135:MET:HG3	1:B:135:MET:HE3	1.84	0.58
1:B:221:THR:HG22	1:B:263:ARG:HE	1.67	0.58
1:B:272:VAL:HA	1:B:291:PHE:CZ	2.39	0.58
1:A:171:GLU:OE2	1:B:147:ARG:NH2	2.36	0.58
4:B:504:CHW:HAE	4:B:504:CHW:OAQ	2.04	0.58
1:B:179:LEU:HD13	1:B:183:ILE:HD12	1.85	0.58
1:B:289:ASN:O	1:B:292:VAL:HG22	2.04	0.58
1:B:89:TYR:OH	1:C:225:ARG:HG3	2.04	0.57
1:D:207:ARG:HH11	1:D:274:HIS:CD2	2.20	0.57
1:B:228:ASP:CG	1:B:256:ARG:HH11	2.08	0.56
4:A:504:CHW:CAE	4:A:504:CHW:OAQ	2.53	0.56
1:A:182:SER:HA	1:A:185:ILE:HG12	1.88	0.56
1:D:71:GLU:OE2	1:D:256:ARG:NH2	2.35	0.56
1:A:60:GLU:HG3	1:A:62:ARG:HH12	1.70	0.56
1:A:187:GLN:HE22	1:B:143:ARG:HH11	1.54	0.55
1:A:209:VAL:HA	1:A:212:LEU:HB2	1.88	0.55
1:C:145:MET:HB3	1:D:170:ILE:HG13	1.88	0.54
1:A:54:VAL:HG21	1:A:242:VAL:HA	1.88	0.54
1:A:145:MET:HB3	1:B:170:ILE:HG13	1.88	0.54
1:A:121:PHE:HE1	4:A:504:CHW:CAT	2.21	0.54
1:D:288:VAL:HG23	5:D:626:HOH:O	2.07	0.54
1:D:54:VAL:CG2	1:D:242:VAL:HG13	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:LEU:HD11	1:D:170:ILE:HG12	1.89	0.54
1:A:135:MET:CE	1:A:136:LEU:HD13	2.34	0.54
1:A:40:ARG:HD3	1:A:43:PHE:CZ	2.43	0.54
1:A:106:ARG:HD3	1:A:107:PHE:H	1.72	0.54
1:A:135:MET:HG3	1:B:135:MET:HE2	1.89	0.53
1:B:207:ARG:HH11	1:B:274:HIS:CD2	2.23	0.53
1:B:77:HIS:NE2	1:C:228:ASP:OD2	2.39	0.53
1:A:97:TRP:O	1:A:101:THR:OG1	2.26	0.53
1:A:262:ILE:O	1:A:266:GLU:HG2	2.09	0.53
1:A:196:VAL:O	1:A:200:ILE:HG12	2.09	0.52
1:C:219:THR:O	1:C:223:VAL:HG23	2.09	0.52
4:B:504:CHW:OAQ	4:B:504:CHW:CAE	2.58	0.52
1:C:110:ILE:HD13	1:C:110:ILE:H	1.74	0.52
1:D:262:ILE:O	1:D:266:GLU:HG2	2.10	0.52
1:C:47:VAL:N	1:C:48:PRO:HD2	2.25	0.51
1:D:136:LEU:O	1:D:140:SER:OG	2.28	0.51
1:A:153:ASN:O	1:A:157:VAL:HG22	2.11	0.51
1:A:135:MET:SD	1:A:135:MET:C	2.89	0.51
1:A:172:LEU:O	1:A:236:LYS:HE3	2.09	0.51
1:D:85:ASP:CG	1:D:207:ARG:HE	2.14	0.51
1:A:54:VAL:HG13	1:A:245:VAL:HG21	1.93	0.50
1:C:177:LEU:O	1:C:181:VAL:HG23	2.12	0.50
1:D:252:ASN:OD1	1:D:252:ASN:N	2.45	0.50
1:B:96:ARG:HH11	1:B:215:GLU:HB3	1.76	0.50
1:D:79:LYS:HG3	1:D:79:LYS:O	2.11	0.49
1:B:113:SER:O	1:B:117:SER:HB2	2.12	0.49
1:B:128:VAL:HB	1:B:129:PRO:HD3	1.95	0.49
1:A:158:GLU:HG3	1:A:269:HIS:CD2	2.47	0.49
1:A:30:THR:N	1:A:31:PRO:CD	2.74	0.49
1:C:143:ARG:HD3	1:D:187:GLN:NE2	2.28	0.48
1:C:280:HIS:CD2	1:C:285:GLN:HG2	2.47	0.48
1:D:129:PRO:O	1:D:132:VAL:HG22	2.13	0.48
1:D:54:VAL:HG22	1:D:242:VAL:HG13	1.93	0.48
1:B:59:SER:N	1:B:160:GLU:OE2	2.38	0.48
1:B:236:LYS:C	1:B:238:ASP:H	2.16	0.48
1:D:121:PHE:HB2	1:D:179:LEU:HD11	1.95	0.48
1:D:163:ARG:O	1:D:167:MET:HG2	2.14	0.48
1:C:166:LEU:O	1:C:170:ILE:HG22	2.14	0.48
1:B:54:VAL:HG22	1:B:242:VAL:HG13	1.96	0.48
1:D:229:GLU:OE2	1:D:231:ARG:NH2	2.47	0.48
1:D:138:HIS:O	1:D:142:LEU:HG	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:LEU:HD22	1:B:33:TRP:CZ3	2.49	0.48
1:B:160:GLU:O	1:B:164:MET:HG2	2.14	0.48
1:C:54:VAL:HG13	1:C:242:VAL:HA	1.94	0.48
1:C:271:VAL:HG12	1:D:40:ARG:O	2.14	0.48
1:A:85:ASP:HA	1:A:207:ARG:HG2	1.97	0.47
1:B:179:LEU:HD13	1:B:183:ILE:CD1	2.44	0.47
1:A:125:VAL:HG21	1:A:186:THR:HG21	1.95	0.47
1:A:167:MET:CE	1:B:147:ARG:HH11	2.27	0.47
1:B:293:VAL:O	1:B:295:LYS:N	2.47	0.47
1:B:46:THR:O	1:B:50:VAL:HG12	2.13	0.47
1:C:135:MET:HG3	1:D:131:MET:HG3	1.98	0.46
1:C:149:LYS:HB2	1:C:288:VAL:HA	1.96	0.46
1:C:119:CYS:O	1:C:123:GLU:HG2	2.15	0.46
1:D:134:GLY:HA3	1:D:156:LEU:HD13	1.98	0.46
1:A:128:VAL:N	1:A:129:PRO:HD2	2.31	0.46
1:A:217:VAL:O	1:A:221:THR:CG2	2.64	0.46
1:A:84:VAL:HB	1:A:203:ARG:NH2	2.30	0.46
1:D:292:VAL:HG23	1:D:293:VAL:HG23	1.98	0.46
1:C:112:GLU:OE1	1:C:232:LEU:HG	2.15	0.46
1:C:147:ARG:HG2	1:D:167:MET:CE	2.46	0.46
1:D:162:GLU:O	1:D:165:HIS:HB2	2.16	0.46
1:B:185:ILE:HD12	1:B:185:ILE:C	2.36	0.45
1:A:125:VAL:HG11	1:A:190:MET:HG3	1.98	0.45
1:A:147:ARG:HG2	1:B:167:MET:HE2	1.98	0.45
1:C:229:GLU:OE1	1:C:231:ARG:HD3	2.16	0.45
1:C:121:PHE:CE1	4:C:504:CHW:HAT	2.40	0.45
1:C:57:GLU:O	1:C:163:ARG:NH1	2.49	0.45
1:C:140:SER:HA	1:C:143:ARG:HG2	1.98	0.45
1:A:260:ASN:ND2	1:A:263:ARG:HH11	2.15	0.45
1:A:207:ARG:HA	1:A:207:ARG:HD3	1.73	0.45
1:D:162:GLU:OE1	3:D:503:OH:O	2.34	0.45
1:A:65:TRP:HB3	1:A:70:ILE:HD13	1.99	0.45
1:B:148:ASP:OD1	1:B:152:ILE:HG13	2.16	0.45
1:C:71:GLU:OE1	1:C:260:ASN:OD1	2.35	0.45
1:A:167:MET:HE1	1:B:147:ARG:HD3	1.96	0.45
1:B:132:VAL:HG23	1:B:136:LEU:CD2	2.47	0.45
1:B:32:VAL:HG13	1:B:32:VAL:O	2.17	0.44
1:A:283:ARG:HA	1:A:285:GLN:HE22	1.82	0.44
1:A:278:ASP:HB3	1:B:44:LEU:HG	1.99	0.44
1:C:262:ILE:O	1:C:266:GLU:HG2	2.17	0.44
1:A:111:THR:OG1	1:A:114:LYS:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:ASP:HB3	1:D:44:LEU:HD12	2.00	0.44
1:C:143:ARG:HH11	1:D:187:GLN:HE22	1.63	0.44
1:B:47:VAL:HB	1:B:48:PRO:HD3	2.00	0.44
1:D:233:ARG:HD3	1:D:233:ARG:N	2.33	0.44
1:D:102:PHE:C	1:D:104:LEU:H	2.22	0.44
1:C:148:ASP:OD1	1:C:151:TRP:HB2	2.17	0.44
1:B:213:GLU:HB3	1:B:266:GLU:O	2.18	0.43
1:D:35:HIS:HA	1:D:38:LEU:HB2	2.00	0.43
1:B:228:ASP:OD2	1:B:256:ARG:NH1	2.40	0.43
1:A:215:GLU:HB3	4:A:504:CHW:HAD	2.00	0.43
1:C:280:HIS:CE1	1:C:285:GLN:HB3	2.53	0.43
1:B:105:TYR:CE1	1:B:118:ARG:HD2	2.53	0.43
1:A:214:GLU:O	1:A:218:ILE:HG13	2.19	0.43
1:A:53:ARG:HH22	1:B:296:LYS:HB2	1.83	0.43
1:C:280:HIS:CD2	1:C:285:GLN:HB3	2.54	0.43
1:B:168:THR:HG21	1:B:258:LEU:HD21	2.00	0.43
1:A:96:ARG:HD2	1:A:215:GLU:OE1	2.19	0.42
1:A:209:VAL:O	1:A:210:GLY:C	2.56	0.42
1:D:203:ARG:HD2	1:D:281:GLU:HB2	2.01	0.42
1:B:122:LEU:HD13	4:B:504:CHW:CAB	2.50	0.42
1:D:244:ARG:HA	1:D:249:LEU:HD12	2.01	0.42
1:A:213:GLU:OE1	1:A:213:GLU:HA	2.19	0.42
1:C:168:THR:O	1:C:171:GLU:HB2	2.19	0.42
1:A:170:ILE:HG12	1:A:170:ILE:O	2.20	0.42
1:C:50:VAL:HG23	1:D:293:VAL:HG21	2.02	0.42
1:A:220:TYR:HB3	1:A:263:ARG:HB2	2.02	0.42
1:C:145:MET:HG2	1:D:166:LEU:HD21	2.01	0.42
1:C:151:TRP:CD1	1:C:289:ASN:HB2	2.55	0.42
1:C:221:THR:HG22	1:C:263:ARG:CZ	2.49	0.41
1:A:162:GLU:O	1:A:165:HIS:HB2	2.21	0.41
1:D:89:TYR:O	1:D:93:ARG:HG2	2.20	0.41
1:A:128:VAL:N	1:A:129:PRO:CD	2.82	0.41
1:A:67:LEU:HB2	1:A:68:PRO:HD3	2.03	0.41
1:A:45:GLU:N	1:A:45:GLU:OE1	2.50	0.41
1:A:203:ARG:NH1	1:A:281:GLU:OE2	2.53	0.41
1:A:135:MET:HG2	1:B:131:MET:HG3	2.02	0.41
1:C:147:ARG:HG2	1:D:167:MET:HE2	2.02	0.41
1:B:132:VAL:HG23	1:B:136:LEU:HD23	2.02	0.41
1:A:267:ALA:O	1:A:271:VAL:HG23	2.20	0.41
1:A:35:HIS:HA	1:A:38:LEU:HB2	2.02	0.41
1:A:187:GLN:NE2	1:B:143:ARG:HH11	2.16	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:GLY:O	1:C:233:ARG:HD3	2.21	0.41
1:A:275:THR:O	1:A:279:MET:HG3	2.21	0.41
1:A:245:VAL:HG23	1:A:246:TYR:N	2.35	0.41
1:A:167:MET:HE2	1:B:147:ARG:NH1	2.34	0.41
1:C:242:VAL:HG22	1:D:147:ARG:HH11	1.86	0.41
1:D:165:HIS:O	1:D:168:THR:HB	2.21	0.41
1:D:63:PRO:HD3	1:D:246:TYR:CZ	2.55	0.41
1:C:35:HIS:CG	1:D:72:ASN:HB3	2.54	0.41
1:B:112:GLU:OE2	1:B:236:LYS:HG2	2.21	0.41
1:C:188:ALA:O	1:C:192:LEU:HB2	2.21	0.40
1:A:78:LYS:HB2	1:B:41:LEU:HD22	2.02	0.40
1:A:166:LEU:HD12	1:B:142:LEU:HA	2.03	0.40
1:A:191:TYR:O	1:A:195:LEU:HB2	2.22	0.40
1:B:214:GLU:OE1	1:B:274:HIS:HE1	2.04	0.40
1:C:280:HIS:NE2	1:C:285:GLN:HB3	2.37	0.40
1:A:206:HIS:O	1:A:273:ASN:HB3	2.22	0.40
1:C:123:GLU:HA	1:C:123:GLU:OE2	2.22	0.40
1:C:92:VAL:O	1:C:95:CYS:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	264/329 (80%)	239 (90%)	25 (10%)	0	100	100
1	B	263/329 (80%)	245 (93%)	16 (6%)	2 (1%)	24	46
1	C	265/329 (80%)	245 (92%)	17 (6%)	3 (1%)	17	36
1	D	264/329 (80%)	248 (94%)	15 (6%)	1 (0%)	39	65
All	All	1056/1316 (80%)	977 (92%)	73 (7%)	6 (1%)	30	56

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	237	ASN
1	B	294	LEU
1	C	173	ARG
1	D	234	PRO
1	C	237	ASN
1	C	236	LYS

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	241/292 (82%)	211 (88%)	30 (12%)	6 11
1	B	240/292 (82%)	215 (90%)	25 (10%)	9 16
1	C	242/292 (83%)	208 (86%)	34 (14%)	4 7
1	D	241/292 (82%)	217 (90%)	24 (10%)	9 18
All	All	964/1168 (82%)	851 (88%)	113 (12%)	7 12

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	THR
1	A	44	LEU
1	A	52	LEU
1	A	96	ARG
1	A	98	LEU
1	A	101	THR
1	A	106	ARG
1	A	107	PHE
1	A	110	ILE
1	A	117	SER
1	A	136	LEU
1	A	140	SER
1	A	146	THR
1	A	156	LEU
1	A	166	LEU
1	A	170	ILE

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Mol	Chain	Res	Type
1	A	179	LEU
1	A	180	ARG
1	A	212	LEU
1	A	221	THR
1	A	225	ARG
1	A	233	ARG
1	A	235	THR
1	A	242	VAL
1	A	252	ASN
1	A	258	LEU
1	A	260	ASN
1	A	263	ARG
1	A	271	VAL
1	A	284	LEU
1	B	40	ARG
1	B	44	LEU
1	B	45	GLU
1	B	49	VAL
1	B	50	VAL
1	B	83	LEU
1	B	87	LEU
1	B	132	VAL
1	B	136	LEU
1	B	156	LEU
1	B	166	LEU
1	B	170	ILE
1	B	177	LEU
1	B	179	LEU
1	B	185	ILE
1	B	192	LEU
1	B	196	VAL
1	B	221	THR
1	B	233	ARG
1	B	242	VAL
1	B	263	ARG
1	B	284	LEU
1	B	285	GLN
1	B	288	VAL
1	B	293	VAL
1	C	44	LEU
1	C	47	VAL
1	C	50	VAL

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Mol	Chain	Res	Type
1	C	52	LEU
1	C	66	SER
1	C	95	CYS
1	C	96	ARG
1	C	104	LEU
1	C	105	TYR
1	C	107	PHE
1	C	110	ILE
1	C	113	SER
1	C	114	LYS
1	C	132	VAL
1	C	146	THR
1	C	156	LEU
1	C	166	LEU
1	C	173	ARG
1	C	179	LEU
1	C	182	SER
1	C	187	GLN
1	C	196	VAL
1	C	225	ARG
1	C	233	ARG
1	C	238	ASP
1	C	239	VAL
1	C	244	ARG
1	C	248	ASN
1	C	260	ASN
1	C	263	ARG
1	C	284	LEU
1	C	285	GLN
1	C	288	VAL
1	C	292	VAL
1	D	52	LEU
1	D	54	VAL
1	D	61	ASP
1	D	72	ASN
1	D	98	LEU
1	D	107	PHE
1	D	110	ILE
1	D	136	LEU
1	D	156	LEU
1	D	166	LEU
1	D	170	ILE

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Mol	Chain	Res	Type
1	D	179	LEU
1	D	185	ILE
1	D	221	THR
1	D	232	LEU
1	D	233	ARG
1	D	238	ASP
1	D	242	VAL
1	D	252	ASN
1	D	260	ASN
1	D	263	ARG
1	D	271	VAL
1	D	284	LEU
1	D	285	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	153	ASN
1	A	187	GLN
1	A	260	ASN
1	A	273	ASN
1	A	274	HIS
1	B	153	ASN
1	B	248	ASN
1	B	269	HIS
1	B	273	ASN
1	B	274	HIS
1	B	285	GLN
1	B	286	ASN
1	C	72	ASN
1	C	77	HIS
1	C	153	ASN
1	C	248	ASN
1	C	260	ASN
1	C	273	ASN
1	C	285	GLN
1	D	81	ASN
1	D	187	GLN
1	D	260	ASN
1	D	273	ASN
1	D	274	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 4 are modelled with single atom and 8 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	CHW	A	504	-	23,24,24	2.29	7 (30%)	30,33,33	1.98	10 (33%)
4	CHW	B	504	-	23,24,24	2.61	9 (39%)	30,33,33	2.04	8 (26%)
4	CHW	C	504	-	23,24,24	2.35	7 (30%)	30,33,33	1.41	4 (13%)
4	CHW	D	504	-	23,24,24	2.30	7 (30%)	30,33,33	1.60	6 (20%)

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	CHW	A	504	-	-	0/17/17/17	0/1/1/1
4	CHW	B	504	-	-	0/17/17/17	0/1/1/1
4	CHW	C	504	-	-	0/17/17/17	0/1/1/1
4	CHW	D	504	-	-	0/17/17/17	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	504	CHW	CAD-CAE	-6.47	1.38	1.50
4	A	504	CHW	CAD-CAE	-6.02	1.39	1.50
4	D	504	CHW	CAD-CAE	-5.89	1.39	1.50
4	C	504	CHW	CAD-CAE	-5.48	1.40	1.50
4	B	504	CHW	CAG-CAH	-4.49	1.38	1.53
4	B	504	CHW	CAH-CAI	-4.19	1.38	1.50
4	A	504	CHW	CAG-CAH	-4.08	1.39	1.53
4	D	504	CHW	CAG-CAH	-4.03	1.39	1.53
4	A	504	CHW	CAH-CAI	-3.97	1.39	1.50
4	C	504	CHW	CAG-CAH	-3.95	1.40	1.53
4	D	504	CHW	CAH-CAI	-3.85	1.39	1.50
4	C	504	CHW	CAH-CAI	-3.67	1.40	1.50
4	B	504	CHW	CAO-CAB	-3.67	1.36	1.40
4	B	504	CHW	CAO-CAU	-3.35	1.36	1.41
4	B	504	CHW	CAP-CAV	-2.47	1.35	1.39
4	B	504	CHW	CAB-CAC	-2.16	1.36	1.40
4	C	504	CHW	CAD-CAC	2.15	1.54	1.51
4	D	504	CHW	CAS-CAJ	2.16	1.54	1.50
4	A	504	CHW	CAS-CAJ	2.45	1.55	1.50
4	A	504	CHW	CAO-CAN	2.51	1.52	1.46
4	C	504	CHW	CAO-CAN	2.56	1.52	1.46
4	D	504	CHW	CAO-CAN	2.59	1.52	1.46
4	A	504	CHW	CAE-CAF	2.59	1.38	1.33
4	B	504	CHW	CAE-CAF	2.80	1.38	1.33
4	D	504	CHW	CAE-CAF	3.29	1.39	1.33
4	C	504	CHW	CAE-CAF	3.59	1.40	1.33
4	B	504	CHW	CAI-CAJ	4.65	1.39	1.33
4	D	504	CHW	CAI-CAJ	5.03	1.39	1.33
4	A	504	CHW	CAI-CAJ	5.08	1.39	1.33
4	C	504	CHW	CAI-CAJ	5.71	1.40	1.33

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	504	CHW	CAP-CAV-CAU	-5.02	118.14	122.56
4	B	504	CHW	CAH-CAI-CAJ	-4.69	122.00	127.17
4	D	504	CHW	CAC-CAD-CAE	-4.20	105.36	112.32
4	A	504	CHW	CAH-CAI-CAJ	-3.49	123.32	127.17
4	A	504	CHW	CAP-CAV-CLAW	-3.49	114.27	117.99
4	C	504	CHW	CAS-CAJ-CAI	-2.90	117.80	123.59
4	D	504	CHW	OAM-CAN-CAO	-2.71	119.63	125.11
4	C	504	CHW	CAP-CAV-CAU	-2.58	120.29	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	504	CHW	OAM-CAN-CAO	-2.39	120.29	125.11
4	C	504	CHW	OAM-CAN-CAO	-2.35	120.37	125.11
4	A	504	CHW	CAP-CAV-CAU	-2.34	120.50	122.56
4	D	504	CHW	CAG-CAF-CAE	-2.27	116.75	121.05
4	A	504	CHW	CAC-CAD-CAE	-2.23	108.63	112.32
4	D	504	CHW	CAP-CAV-CAU	-2.15	120.66	122.56
4	A	504	CHW	OAQ-CAP-CAV	-2.14	114.06	120.50
4	B	504	CHW	CAC-CAD-CAE	-2.13	108.78	112.32
4	B	504	CHW	CAU-CAO-CAN	-2.09	118.74	121.78
4	A	504	CHW	CAU-CAO-CAN	-2.07	118.77	121.78
4	B	504	CHW	OAM-CAN-CAO	-2.01	121.05	125.11
4	D	504	CHW	CAS-CAJ-CAK	2.54	121.77	115.86
4	A	504	CHW	CAG-CAH-CAI	2.68	118.71	111.69
4	B	504	CHW	CAR-CAF-CAG	2.89	119.82	115.41
4	B	504	CHW	CAG-CAH-CAI	3.56	121.02	111.69
4	C	504	CHW	CAR-CAF-CAG	3.82	121.24	115.41
4	D	504	CHW	CAR-CAF-CAG	3.84	121.28	115.41
4	A	504	CHW	CAR-CAF-CAG	4.21	121.84	115.41
4	B	504	CHW	CAU-CAV-CLAW	4.30	125.16	118.66
4	A	504	CHW	CAU-CAV-CLAW	4.34	125.23	118.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	504	CHW	3	0
4	B	504	CHW	3	0
4	C	504	CHW	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	266/329 (80%)	0.51	10 (3%) 44 36	22, 37, 56, 91	0
1	B	265/329 (80%)	0.44	6 (2%) 64 57	21, 37, 52, 63	0
1	C	266/329 (80%)	0.70	19 (7%) 19 13	26, 44, 78, 113	0
1	D	266/329 (80%)	0.80	27 (10%) 9 5	27, 44, 77, 112	0
All	All	1063/1316 (80%)	0.61	62 (5%) 26 20	21, 40, 65, 113	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	106	ARG	6.9
1	C	108	GLY	6.9
1	D	109	SER	6.5
1	C	109	SER	6.2
1	C	107	PHE	6.1
1	D	235	THR	5.7
1	C	110	ILE	5.7
1	D	106	ARG	5.3
1	D	107	PHE	4.8
1	D	105	TYR	4.7
1	D	173	ARG	4.2
1	D	179	LEU	4.0
1	C	184	ILE	3.9
1	A	293	VAL	3.8
1	D	30	THR	3.7
1	D	253	ALA	3.6
1	C	31	PRO	3.6
1	A	30	THR	3.5
1	C	116	ILE	3.5
1	D	115	VAL	3.5
1	C	239	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	234	PRO	3.4
1	A	238	ASP	3.4
1	D	236	LYS	3.4
1	A	235	THR	3.3
1	D	110	ILE	3.3
1	D	50	VAL	3.2
1	A	81	ASN	3.2
1	C	235	THR	3.2
1	D	208	PHE	3.0
1	D	108	GLY	3.0
1	C	97	TRP	2.9
1	C	112	GLU	2.9
1	B	45	GLU	2.9
1	D	52	LEU	2.8
1	A	107	PHE	2.6
1	B	46	THR	2.6
1	B	181	VAL	2.6
1	C	245	VAL	2.6
1	D	234	PRO	2.6
1	C	111	THR	2.6
1	C	98	LEU	2.5
1	D	242	VAL	2.5
1	D	177	LEU	2.5
1	A	232	LEU	2.5
1	D	258	LEU	2.4
1	B	223	VAL	2.4
1	D	192	LEU	2.4
1	D	238	ASP	2.4
1	A	31	PRO	2.3
1	D	97	TRP	2.3
1	D	48	PRO	2.2
1	C	291	PHE	2.2
1	C	122	LEU	2.2
1	B	239	VAL	2.1
1	D	204	PHE	2.1
1	B	275	THR	2.1
1	A	192	LEU	2.1
1	D	144	TYR	2.0
1	C	102	PHE	2.0
1	D	124	THR	2.0
1	C	91	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	CHW	D	504	24/24	0.93	0.36	3.70	49,54,57,61	0
2	FE	D	502	1/1	0.97	0.21	2.35	35,35,35,35	0
2	FE	B	502	1/1	0.99	0.20	2.01	32,32,32,32	0
4	CHW	A	504	24/24	0.91	0.23	2.00	25,36,45,49	0
4	CHW	C	504	24/24	0.87	0.30	1.99	43,52,59,64	0
3	OH	B	503	1/1	0.99	0.18	1.19	17,17,17,17	0
4	CHW	B	504	24/24	0.94	0.18	0.73	31,40,57,58	0
2	FE	C	501	1/1	0.97	0.19	0.41	46,46,46,46	0
2	FE	C	502	1/1	0.99	0.17	0.40	39,39,39,39	0
2	FE	A	502	1/1	0.99	0.18	0.22	32,32,32,32	0
2	FE	A	501	1/1	0.99	0.15	-0.17	31,31,31,31	0
3	OH	C	503	1/1	1.00	0.15	-0.67	12,12,12,12	0
3	OH	A	503	1/1	1.00	0.15	-0.68	16,16,16,16	0
2	FE	B	501	1/1	0.99	0.14	-0.75	30,30,30,30	0
3	OH	D	503	1/1	0.99	0.15	-0.93	13,13,13,13	0
2	FE	D	501	1/1	1.00	0.12	-2.65	43,43,43,43	0

6.5 Other polymers (i)

There are no such residues in this entry.