Full wwPDB X-ray Structure Validation Report (i)

Mar 9, 2024 – 12:35 PM EST

PDB ID	:	3VV9
Title	:	Crystal structure of cyanide-insensitive alternative oxidase from Trypanosoma brucei
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	:	2.85 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

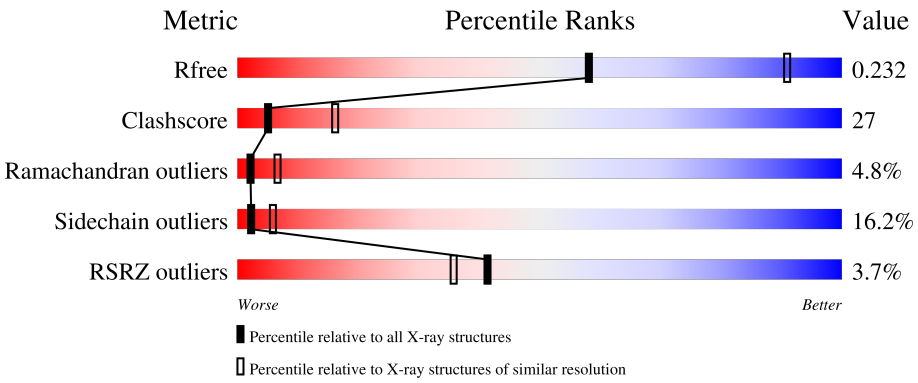
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.85 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}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	% 37% 37% 7% • 19%
1	B	329	4% 39% 35% 7% • 19%
1	C	329	3% 35% 36% 10% • 19%
1	D	329	4% 38% 34% 9% 19%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8718 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.

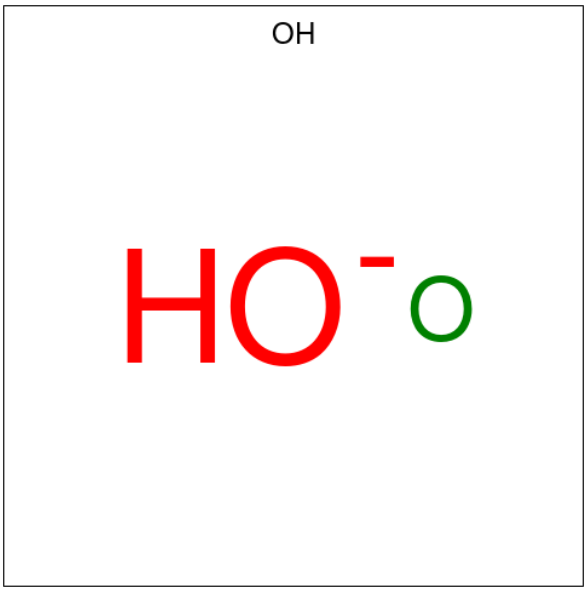
- Molecule 1 is a protein called Alternative oxidase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	267	2170	1390	386	384	10	0	0	0
1	B	268	2179	1395	387	387	10	0	0	0
1	C	266	2163	1385	385	383	10	0	0	0
1	D	266	2163	1385	385	383	10	0	0	0

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

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

- 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 water.

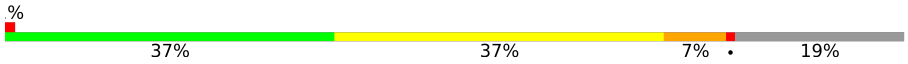
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	14	Total O 14 14	0	0
4	B	8	Total O 8 8	0	0
4	C	7	Total O 7 7	0	0
4	D	2	Total O 2 2	0	0

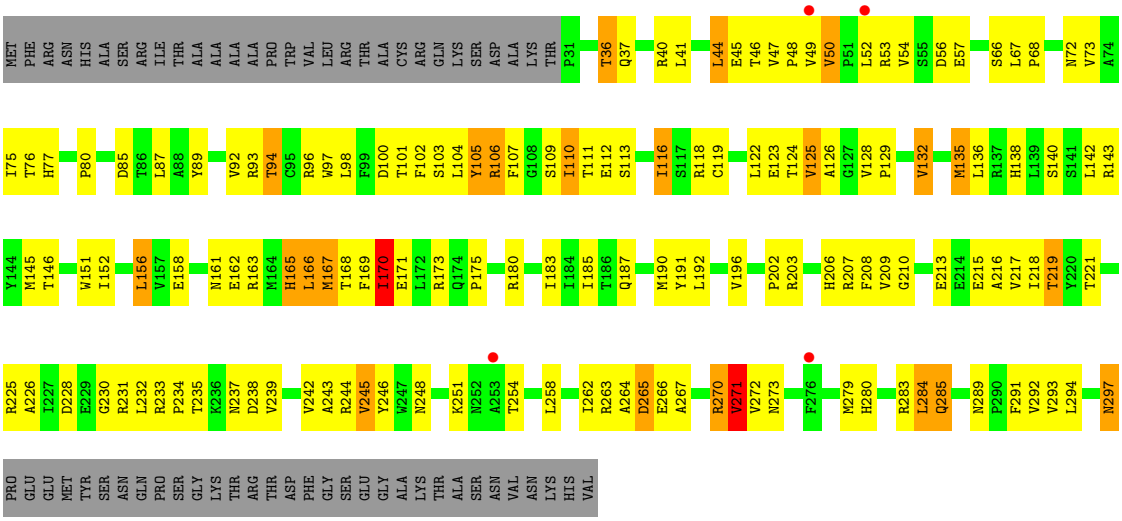
3 Residue-property plots (i)

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

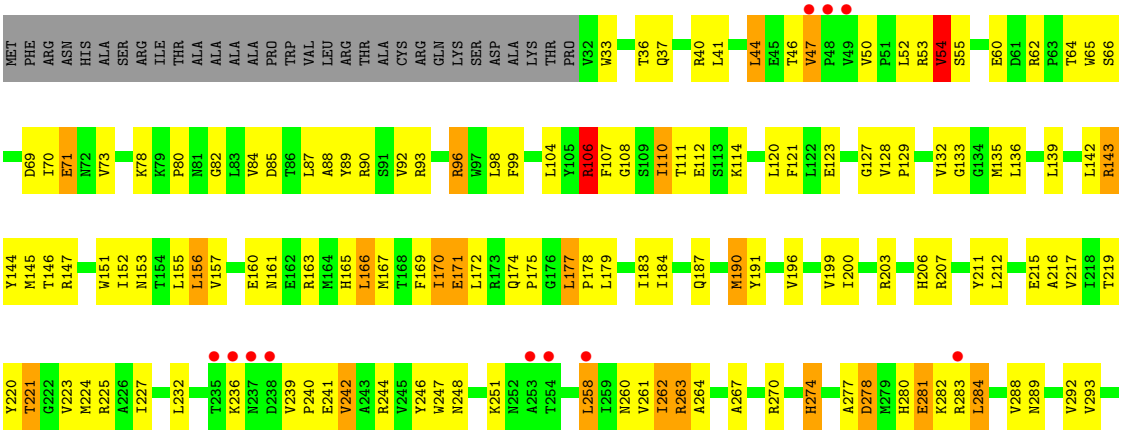
Chain A:

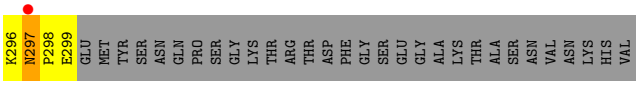




• Molecule 1: Alternative oxidase, mitochondrial

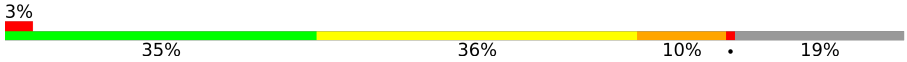
Chain B:

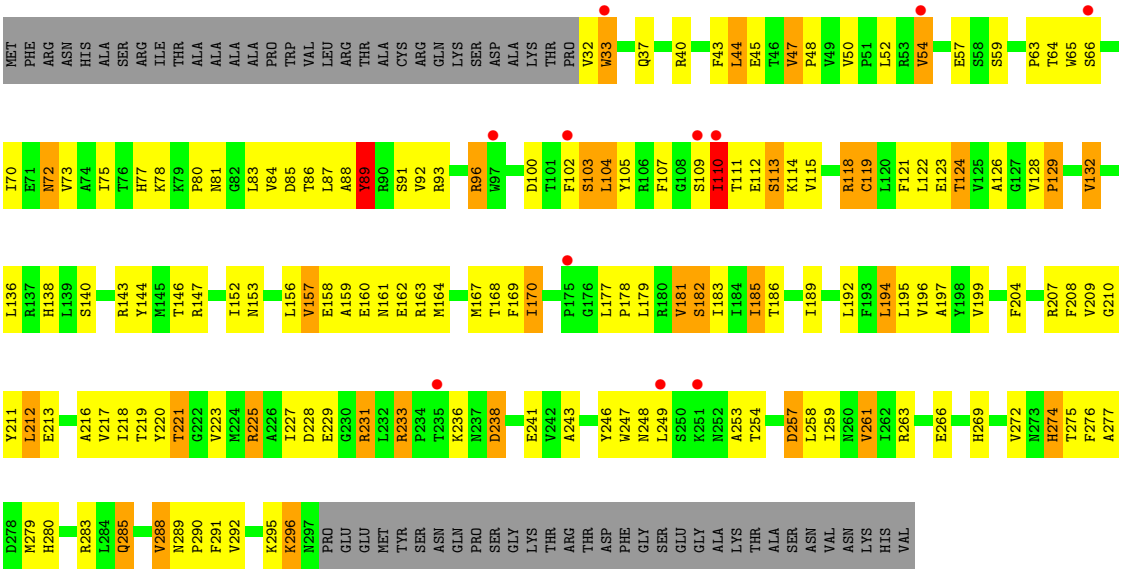




• Molecule 1: Alternative oxidase, mitochondrial

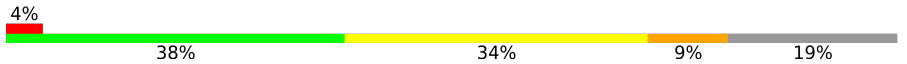
Chain C:

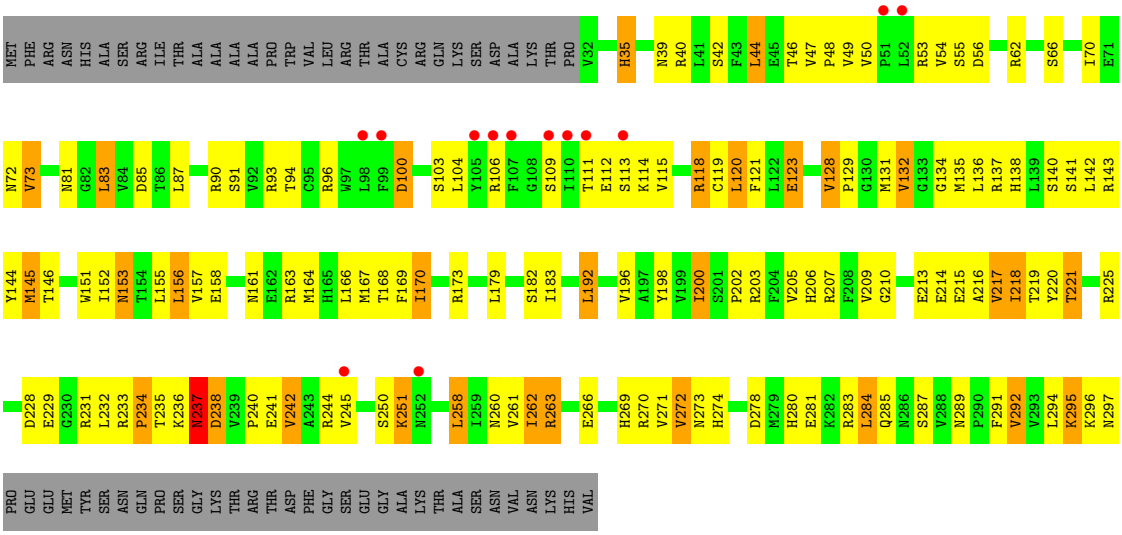




• Molecule 1: Alternative oxidase, mitochondrial

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	261.31Å 63.12Å 136.46Å 90.00° 121.38° 90.00°	Depositor
Resolution (Å)	45.38 – 2.85 45.38 – 2.85	Depositor EDS
% Data completeness (in resolution range)	87.6 (45.38-2.85) 90.4 (45.38-2.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.32 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.192 , 0.247 0.191 , 0.232	Depositor DCC
R_{free} test set	1998 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å^2)	86.9	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 79.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.157 for -h-2*l,-k,l	Xtriage
Reported twinning fraction	0.524 for H, K, L 0.476 for H+4/2L, -K, -L	Depositor
Outliers	1 of 40879 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8718	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.68% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.50	0/2220	0.78	1/3015 (0.0%)
1	B	0.53	0/2229	0.79	3/3028 (0.1%)
1	C	0.47	0/2212	0.73	0/3004
1	D	0.50	0/2212	0.75	0/3004
All	All	0.50	0/8873	0.76	4/12051 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	278	ASP	CB-CG-OD1	5.57	123.31	118.30
1	B	52	LEU	CA-CB-CG	5.46	127.85	115.30
1	A	156	LEU	CA-CB-CG	5.19	127.25	115.30
1	B	108	GLY	N-CA-C	-5.10	100.34	113.10

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	2170	0	2202	143	0
1	B	2179	0	2207	143	0
1	C	2163	0	2194	113	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2163	0	2194	122	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
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	14	0	0	3	0
4	B	8	0	0	0	0
4	C	7	0	0	2	0
4	D	2	0	0	0	0
All	All	8718	0	8797	473	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 27.

All (473) 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:C:163:ARG:O	1:C:167:MET:HG2	1.46	1.13
1:D:295:LYS:HB2	1:D:295:LYS:NZ	1.62	1.12
1:B:297:ASN:HB2	1:B:298:PRO:CD	1.86	1.05
1:A:170:ILE:HG13	1:B:145:MET:HB3	1.05	1.04
1:D:295:LYS:HB2	1:D:295:LYS:HZ3	1.20	1.02
1:D:168:THR:HG23	1:D:240:PRO:HG3	1.42	1.01
1:A:170:ILE:HG13	1:B:145:MET:CB	1.92	1.00
1:C:123:GLU:HG3	1:C:169:PHE:HE2	1.30	0.95
1:C:233:ARG:H	1:C:233:ARG:HD2	1.32	0.95
1:B:282:LYS:O	1:B:284:LEU:HD13	1.65	0.94
1:B:297:ASN:HB2	1:B:298:PRO:HD2	1.52	0.90
1:C:123:GLU:HG3	1:C:169:PHE:CE2	2.09	0.88
1:A:119:CYS:O	1:A:123:GLU:HG2	1.76	0.85
1:A:167:MET:HE2	1:B:147:ARG:HA	1.59	0.85
1:D:54:VAL:HG11	1:D:242:VAL:HA	1.58	0.85
1:C:54:VAL:HG11	1:C:241:GLU:HG2	1.59	0.84
1:A:187:GLN:HE22	1:B:143:ARG:NH1	1.75	0.84
1:D:295:LYS:HZ3	1:D:295:LYS:CB	1.92	0.83
1:A:170:ILE:CG1	1:B:145:MET:HB3	2.01	0.83
1:C:231:ARG:HH21	1:C:231:ARG:HG3	1.42	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:VAL:O	1:C:221:THR:HG22	1.79	0.83
1:D:168:THR:HG23	1:D:240:PRO:CG	2.09	0.82
1:A:151:TRP:HZ2	1:A:279:MET:HE2	1.45	0.82
1:A:167:MET:CE	1:B:147:ARG:HD3	2.10	0.81
1:A:283:ARG:HA	1:A:285:GLN:HE22	1.45	0.79
1:D:123:GLU:OE2	1:D:123:GLU:HA	1.80	0.79
1:A:213:GLU:OE1	1:A:213:GLU:HA	1.80	0.79
1:B:89:TYR:O	1:B:93:ARG:HG2	1.83	0.79
1:D:96:ARG:O	1:D:100:ASP:HB2	1.82	0.79
1:A:192:LEU:O	1:A:196:VAL:HG12	1.84	0.77
1:D:217:VAL:O	1:D:221:THR:HG22	1.82	0.77
1:B:54:VAL:HG22	1:B:242:VAL:HG13	1.67	0.76
1:B:297:ASN:CB	1:B:298:PRO:CD	2.63	0.76
1:C:231:ARG:HH21	1:C:231:ARG:CG	1.98	0.76
1:C:110:ILE:O	1:C:110:ILE:HG23	1.86	0.75
1:A:283:ARG:HA	1:A:285:GLN:NE2	2.00	0.75
1:B:207:ARG:HD3	1:B:274:HIS:CD2	2.22	0.75
1:B:207:ARG:NH1	1:B:277:ALA:HB3	2.02	0.75
1:A:151:TRP:CZ2	1:A:279:MET:HE2	2.22	0.73
1:B:207:ARG:HH11	1:B:274:HIS:HD2	1.36	0.73
1:D:111:THR:C	1:D:113:SER:H	1.91	0.73
1:A:202:PRO:HD2	4:A:606:HOH:O	1.89	0.72
1:A:75:ILE:HG12	1:A:218:ILE:HG12	1.69	0.72
1:A:93:ARG:NH2	1:A:215:GLU:OE2	2.22	0.72
1:A:44:LEU:HG	1:B:278:ASP:HB3	1.72	0.72
1:B:104:LEU:HB3	1:B:106:ARG:NH2	2.05	0.72
1:D:118:ARG:HG2	1:D:119:CYS:N	2.04	0.72
1:D:196:VAL:O	1:D:200:ILE:HG12	1.87	0.72
1:D:295:LYS:HB2	1:D:295:LYS:HZ2	1.51	0.72
1:C:168:THR:HG23	1:C:243:ALA:HB2	1.71	0.71
1:B:104:LEU:HB3	1:B:106:ARG:HH21	1.54	0.71
1:C:143:ARG:HG3	1:C:144:TYR:CD2	2.26	0.71
1:A:167:MET:CE	1:B:147:ARG:HA	2.21	0.71
1:B:297:ASN:HB2	1:B:298:PRO:HD3	1.72	0.70
1:A:166:LEU:HD12	1:B:142:LEU:HD23	1.73	0.70
1:A:167:MET:HE2	1:B:147:ARG:HD3	1.71	0.70
1:B:296:LYS:HG3	1:B:297:ASN:N	2.07	0.70
1:C:126:ALA:HB1	1:C:162:GLU:OE2	1.92	0.70
1:C:65:TRP:HD1	1:C:261:VAL:HG12	1.57	0.69
1:A:217:VAL:O	1:A:221:THR:HG22	1.91	0.69
1:B:54:VAL:CG2	1:B:242:VAL:HG13	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:THR:HG21	1:A:183:ILE:HG12	1.75	0.69
1:A:135:MET:HE3	1:B:135:MET:HG3	1.73	0.68
1:A:170:ILE:O	1:A:170:ILE:HG23	1.93	0.68
1:A:151:TRP:HZ2	1:A:279:MET:CE	2.06	0.68
1:B:66:SER:O	1:B:69:ASP:HB3	1.94	0.68
1:D:134:GLY:HA3	1:D:156:LEU:CD1	2.24	0.68
1:B:89:TYR:CZ	1:B:93:ARG:HD3	2.29	0.67
1:A:123:GLU:HA	1:A:126:ALA:HB3	1.77	0.67
1:C:119:CYS:HA	1:C:122:LEU:HD12	1.76	0.67
1:B:278:ASP:O	1:B:282:LYS:HG2	1.95	0.67
1:D:54:VAL:CG1	1:D:242:VAL:HA	2.25	0.66
1:C:104:LEU:HD23	1:C:107:PHE:HB3	1.76	0.66
1:D:132:VAL:O	1:D:136:LEU:HD13	1.95	0.66
1:D:202:PRO:HB2	1:D:280:HIS:NE2	2.10	0.66
1:D:168:THR:CG2	1:D:240:PRO:HG3	2.22	0.66
1:C:123:GLU:CG	1:C:169:PHE:HE2	2.05	0.66
1:C:195:LEU:O	1:C:199:VAL:HG23	1.96	0.66
1:A:145:MET:SD	1:B:175:PRO:HG3	2.35	0.65
1:C:229:GLU:OE1	1:C:231:ARG:NH2	2.30	0.65
1:D:294:LEU:O	1:D:295:LYS:HB2	1.96	0.65
1:C:143:ARG:HG3	1:C:144:TYR:HD2	1.62	0.65
1:C:280:HIS:CD2	1:C:285:GLN:HG2	2.32	0.65
1:C:96:ARG:HG3	1:C:96:ARG:HH11	1.59	0.65
1:A:289:ASN:O	1:A:292:VAL:HG22	1.96	0.65
1:B:179:LEU:O	1:B:183:ILE:HD12	1.96	0.65
1:B:217:VAL:O	1:B:221:THR:HG23	1.97	0.64
1:A:76:THR:H	1:A:270:ARG:NH1	1.96	0.63
1:C:96:ARG:HG3	1:C:96:ARG:NH1	2.13	0.63
1:B:282:LYS:HB2	1:B:284:LEU:HD22	1.80	0.63
1:A:202:PRO:HG2	1:A:280:HIS:NE2	2.14	0.63
1:A:125:VAL:CG1	1:A:190:MET:HG3	2.29	0.63
1:D:284:LEU:O	1:D:287:SER:HB2	1.98	0.63
1:A:41:LEU:HD22	1:B:78:LYS:CA	2.29	0.62
1:A:202:PRO:HG2	1:A:280:HIS:CD2	2.34	0.62
1:D:120:LEU:HD11	1:D:170:ILE:HG12	1.80	0.62
1:A:125:VAL:HG11	1:A:190:MET:HG3	1.81	0.62
1:B:36:THR:HB	1:B:37:GLN:OE1	1.98	0.62
1:B:239:VAL:HG22	1:B:258:LEU:HD12	1.82	0.62
1:C:65:TRP:CD1	1:C:261:VAL:HG12	2.34	0.62
1:D:217:VAL:C	1:D:221:THR:HG22	2.18	0.62
1:A:294:LEU:HD23	1:B:33:TRP:CE3	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:ARG:NH2	1:D:42:SER:O	2.33	0.62
1:A:44:LEU:O	1:A:47:VAL:HG13	2.00	0.61
1:A:122:LEU:O	1:A:125:VAL:HG23	2.00	0.61
1:A:151:TRP:CZ2	1:A:279:MET:CE	2.83	0.61
1:B:73:VAL:HB	1:B:263:ARG:NH1	2.14	0.61
1:D:55:SER:O	1:D:62:ARG:NH2	2.34	0.61
1:D:83:LEU:O	1:D:87:LEU:N	2.31	0.61
1:B:104:LEU:CB	1:B:106:ARG:HH21	2.13	0.60
1:B:203:ARG:HD2	1:B:281:GLU:HB2	1.83	0.60
1:A:285:GLN:CD	1:A:285:GLN:H	2.03	0.60
1:B:172:LEU:HA	1:B:236:LYS:HE2	1.83	0.60
1:C:257:ASP:OD2	1:C:257:ASP:N	2.30	0.60
1:D:241:GLU:HG2	1:D:244:ARG:HH21	1.66	0.60
1:B:196:VAL:O	1:B:200:ILE:HG12	2.01	0.60
1:C:236:LYS:HE3	4:C:605:HOH:O	2.01	0.60
1:A:191:TYR:HE2	1:B:135:MET:HE1	1.67	0.60
1:D:217:VAL:HG21	1:D:270:ARG:HH11	1.67	0.60
1:B:54:VAL:HG22	1:B:242:VAL:CG1	2.31	0.60
1:C:118:ARG:HH11	1:C:118:ARG:HG3	1.67	0.60
1:B:246:TYR:HD2	1:B:247:TRP:CE3	2.20	0.60
1:A:41:LEU:HD22	1:B:78:LYS:HA	1.83	0.59
1:D:272:VAL:HG12	1:D:273:ASN:N	2.18	0.59
1:C:275:THR:O	1:C:279:MET:HG3	2.03	0.59
1:A:36:THR:HG22	1:A:37:GLN:NE2	2.18	0.59
1:A:170:ILE:O	1:A:170:ILE:CG2	2.50	0.59
1:C:118:ARG:HG3	1:C:118:ARG:NH1	2.17	0.59
1:C:161:ASN:OD1	1:C:269:HIS:HE1	1.85	0.59
1:C:164:MET:HG3	1:C:246:TYR:CE1	2.38	0.59
1:A:128:VAL:HB	1:A:129:PRO:HD3	1.85	0.59
1:B:82:GLY:HA3	1:B:203:ARG:HH22	1.67	0.59
1:A:264:ALA:O	1:A:265:ASP:C	2.42	0.58
1:A:96:ARG:HD2	1:A:215:GLU:OE1	2.04	0.58
1:A:297:ASN:N	1:A:297:ASN:HD22	2.02	0.58
1:B:41:LEU:HG	1:C:72:ASN:ND2	2.17	0.58
1:D:70:ILE:O	1:D:73:VAL:HB	2.03	0.58
1:D:217:VAL:HG21	1:D:270:ARG:NH1	2.18	0.58
1:A:76:THR:H	1:A:270:ARG:HH12	1.49	0.58
1:A:135:MET:CE	1:B:135:MET:HE2	2.34	0.58
1:A:143:ARG:HD3	1:B:187:GLN:NE2	2.19	0.58
1:A:209:VAL:HG11	1:A:273:ASN:OD1	2.04	0.58
1:C:59:SER:HB3	1:C:160:GLU:OE1	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:ARG:HD2	1:B:107:PHE:H	1.67	0.57
1:A:167:MET:HE3	1:B:147:ARG:HD3	1.86	0.57
1:C:207:ARG:HH11	1:C:274:HIS:HD2	1.52	0.57
1:A:187:GLN:HE22	1:B:143:ARG:HH11	1.51	0.57
1:D:115:VAL:HA	1:D:118:ARG:HB3	1.86	0.57
1:D:134:GLY:HA3	1:D:156:LEU:HD13	1.85	0.57
1:B:93:ARG:HE	1:D:229:GLU:CD	2.08	0.57
1:B:112:GLU:CA	1:B:232:LEU:HD11	2.35	0.57
1:A:46:THR:O	1:A:50:VAL:HG12	2.04	0.57
1:D:234:PRO:O	1:D:237:ASN:HB2	2.04	0.57
1:D:294:LEU:O	1:D:295:LYS:CB	2.52	0.57
1:A:67:LEU:N	1:A:68:PRO:HD2	2.19	0.57
1:C:92:VAL:HG22	1:C:208:PHE:CD1	2.40	0.57
1:C:213:GLU:O	1:C:217:VAL:HG23	2.03	0.57
1:D:237:ASN:O	1:D:237:ASN:ND2	2.37	0.57
1:A:146:THR:C	1:B:167:MET:HE1	2.25	0.56
1:B:37:GLN:OE1	1:B:37:GLN:N	2.33	0.56
1:B:96:ARG:NH1	1:B:215:GLU:HB3	2.20	0.56
1:B:199:VAL:HG12	1:B:200:ILE:HD13	1.87	0.56
1:C:153:ASN:O	1:C:157:VAL:HG23	2.06	0.56
1:C:161:ASN:OD1	1:C:269:HIS:CE1	2.58	0.56
1:B:123:GLU:OE2	1:B:123:GLU:HA	2.06	0.56
1:B:90:ARG:HD3	1:D:229:GLU:O	2.06	0.56
1:C:81:ASN:N	1:C:85:ASP:OD2	2.38	0.56
1:C:272:VAL:HA	1:C:291:PHE:CZ	2.41	0.56
1:C:289:ASN:O	1:C:292:VAL:HG22	2.05	0.56
1:A:44:LEU:HD11	1:B:282:LYS:HG3	1.88	0.56
1:A:89:TYR:OH	1:C:225:ARG:HG3	2.06	0.56
1:B:155:LEU:HD21	1:B:206:HIS:HE1	1.69	0.56
1:B:297:ASN:CB	1:B:298:PRO:HD3	2.34	0.56
1:D:235:THR:C	1:D:237:ASN:H	2.09	0.55
1:A:170:ILE:HG21	1:B:145:MET:O	2.05	0.55
1:B:85:ASP:CG	1:B:207:ARG:HE	2.09	0.55
1:C:170:ILE:HD13	1:C:170:ILE:O	2.07	0.55
1:C:233:ARG:HD2	1:C:233:ARG:N	2.12	0.55
1:D:93:ARG:HH21	1:D:96:ARG:HH11	1.54	0.55
1:C:100:ASP:OD1	1:C:118:ARG:NH1	2.40	0.55
1:A:135:MET:HE3	1:B:135:MET:HE2	1.89	0.54
1:A:234:PRO:HB2	1:A:237:ASN:HD21	1.71	0.54
1:B:96:ARG:NH2	1:B:219:THR:OG1	2.39	0.54
1:C:96:ARG:HH11	1:C:96:ARG:CG	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:TYR:CE2	1:B:135:MET:HE1	2.42	0.54
1:A:123:GLU:HA	1:A:126:ALA:CB	2.37	0.54
1:B:144:TYR:O	1:B:146:THR:HG23	2.08	0.54
1:D:153:ASN:O	1:D:157:VAL:HG13	2.08	0.54
1:D:203:ARG:HD2	1:D:281:GLU:HB2	1.89	0.54
1:C:168:THR:CG2	1:C:243:ALA:HB2	2.38	0.54
1:D:47:VAL:N	1:D:48:PRO:CD	2.71	0.54
1:A:103:SER:O	1:A:104:LEU:HB2	2.08	0.54
1:A:166:LEU:CD1	1:B:142:LEU:HA	2.37	0.54
1:B:123:GLU:OE1	1:B:220:TYR:OH	2.26	0.54
1:B:190:MET:O	1:B:191:TYR:C	2.45	0.54
1:B:221:THR:HG22	1:B:263:ARG:HE	1.72	0.54
1:C:129:PRO:O	1:C:132:VAL:N	2.40	0.54
1:D:258:LEU:HD23	1:D:262:ILE:HG13	1.89	0.54
1:C:40:ARG:HD3	1:C:43:PHE:CZ	2.42	0.53
1:D:258:LEU:HD23	1:D:258:LEU:C	2.27	0.53
1:A:266:GLU:OE2	1:A:266:GLU:HA	2.08	0.53
1:B:44:LEU:O	1:B:47:VAL:HG13	2.07	0.53
1:A:85:ASP:HA	1:A:207:ARG:HG2	1.90	0.53
1:A:94:THR:O	1:A:97:TRP:HB3	2.09	0.53
1:A:294:LEU:HD23	1:B:33:TRP:CZ3	2.43	0.53
1:C:229:GLU:OE1	1:C:231:ARG:HG3	2.08	0.53
1:D:90:ARG:O	1:D:93:ARG:HB2	2.09	0.53
1:C:182:SER:O	1:C:186:THR:OG1	2.24	0.53
1:D:46:THR:O	1:D:49:VAL:HG22	2.09	0.53
1:D:111:THR:HB	1:D:114:LYS:H	1.74	0.53
1:D:140:SER:OG	1:D:143:ARG:NH2	2.42	0.53
1:D:119:CYS:C	1:D:121:PHE:H	2.13	0.52
1:D:198:TYR:O	1:D:202:PRO:HG3	2.09	0.52
1:D:111:THR:C	1:D:113:SER:N	2.61	0.52
1:D:215:GLU:O	1:D:218:ILE:HB	2.09	0.52
1:C:110:ILE:O	1:C:110:ILE:CG2	2.57	0.52
1:A:175:PRO:HG2	1:A:180:ARG:HG3	1.91	0.52
1:B:54:VAL:HG11	1:B:241:GLU:HG2	1.91	0.52
1:C:158:GLU:O	1:C:161:ASN:HB3	2.10	0.52
1:B:120:LEU:HD21	1:B:175:PRO:HD3	1.92	0.52
1:B:167:MET:O	1:B:170:ILE:HG22	2.08	0.52
1:B:139:LEU:HB3	1:B:143:ARG:HH12	1.73	0.52
1:C:123:GLU:OE1	1:C:220:TYR:OH	2.28	0.52
1:D:142:LEU:O	1:D:145:MET:N	2.33	0.52
1:D:213:GLU:O	1:D:214:GLU:C	2.48	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:MET:O	1:A:135:MET:HG2	2.10	0.52
1:A:262:ILE:O	1:A:266:GLU:HG2	2.10	0.52
1:C:209:VAL:HA	1:C:212:LEU:HB2	1.92	0.52
1:D:113:SER:HA	1:D:173:ARG:HD3	1.91	0.52
1:D:128:VAL:H	1:D:129:PRO:CD	2.23	0.52
1:D:134:GLY:HA3	1:D:156:LEU:HD11	1.91	0.52
1:C:88:ALA:HA	1:C:204:PHE:CE1	2.44	0.52
1:C:247:TRP:CD1	1:C:261:VAL:HB	2.45	0.52
1:D:161:ASN:O	1:D:164:MET:N	2.43	0.52
1:D:155:LEU:HD21	1:D:206:HIS:HE1	1.74	0.51
1:D:283:ARG:HA	1:D:285:GLN:NE2	2.25	0.51
1:C:296:LYS:HD2	1:C:296:LYS:O	2.10	0.51
1:A:76:THR:N	1:A:270:ARG:HH12	2.08	0.51
1:D:296:LYS:O	1:D:297:ASN:HB3	2.10	0.51
1:B:220:TYR:HB2	1:B:263:ARG:HB2	1.91	0.51
1:D:258:LEU:HD23	1:D:258:LEU:O	2.11	0.51
1:A:96:ARG:HH12	1:A:118:ARG:HH21	1.58	0.51
1:A:221:THR:HB	1:A:263:ARG:HE	1.75	0.51
1:C:181:VAL:O	1:C:183:ILE:N	2.44	0.51
1:D:236:LYS:C	1:D:238:ASP:N	2.64	0.51
1:B:171:GLU:OE1	1:B:240:PRO:HB3	2.11	0.51
1:A:166:LEU:HD21	1:B:145:MET:HG2	1.93	0.50
1:C:103:SER:HB2	1:C:105:TYR:HB2	1.94	0.50
1:C:121:PHE:O	1:C:124:THR:HG23	2.11	0.50
1:A:47:VAL:N	1:A:48:PRO:CD	2.73	0.50
1:B:80:PRO:CB	1:B:85:ASP:HB3	2.41	0.50
1:C:288:VAL:HG13	1:C:289:ASN:N	2.26	0.50
1:A:106:ARG:HD3	1:A:107:PHE:HD1	1.77	0.50
1:A:239:VAL:CG1	1:A:244:ARG:HG3	2.42	0.50
1:D:35:HIS:HD2	1:D:39:ASN:ND2	2.09	0.50
1:A:75:ILE:HG12	1:A:218:ILE:CG1	2.39	0.50
1:A:116:ILE:HG21	1:A:173:ARG:HB3	1.93	0.50
1:D:144:TYR:O	1:D:146:THR:HG23	2.11	0.50
1:D:213:GLU:O	1:D:216:ALA:N	2.45	0.50
1:D:262:ILE:O	1:D:266:GLU:HG2	2.12	0.50
1:C:37:GLN:H	1:C:37:GLN:CD	2.15	0.49
1:A:225:ARG:NH1	1:A:228:ASP:OD2	2.46	0.49
1:A:218:ILE:HA	1:A:221:THR:CG2	2.42	0.49
1:D:118:ARG:CG	1:D:119:CYS:N	2.74	0.49
1:B:44:LEU:C	1:B:44:LEU:CD2	2.81	0.49
1:B:207:ARG:HD3	1:B:274:HIS:HD2	1.72	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:LEU:O	1:D:196:VAL:HG13	2.12	0.49
1:A:53:ARG:HB2	1:A:56:ASP:OD2	2.13	0.49
1:A:135:MET:CE	1:B:135:MET:CE	2.90	0.49
1:A:226:ALA:O	1:A:230:GLY:N	2.44	0.49
1:D:73:VAL:HG11	1:D:263:ARG:HD3	1.95	0.49
1:C:143:ARG:HG3	1:C:144:TYR:CE2	2.47	0.49
1:D:128:VAL:H	1:D:129:PRO:HD2	1.76	0.49
1:D:237:ASN:C	1:D:237:ASN:HD22	2.16	0.49
1:C:47:VAL:HA	1:C:50:VAL:HG12	1.95	0.48
1:D:217:VAL:O	1:D:218:ILE:C	2.51	0.48
1:A:280:HIS:CE1	1:A:285:GLN:HB3	2.48	0.48
1:D:225:ARG:O	1:D:228:ASP:N	2.44	0.48
1:B:112:GLU:HA	1:B:232:LEU:HD11	1.95	0.48
1:B:112:GLU:N	1:B:232:LEU:HD11	2.29	0.48
1:C:296:LYS:O	1:C:296:LYS:HG3	2.14	0.48
1:A:162:GLU:O	1:A:165:HIS:HB2	2.13	0.48
1:C:33:TRP:CD1	1:C:33:TRP:O	2.67	0.48
1:C:296:LYS:O	1:C:296:LYS:CG	2.61	0.48
1:A:128:VAL:O	1:A:132:VAL:HG13	2.14	0.48
1:C:192:LEU:O	1:C:196:VAL:HG13	2.13	0.48
1:C:220:TYR:CE2	1:C:266:GLU:HG3	2.49	0.48
1:D:161:ASN:O	1:D:164:MET:HB2	2.14	0.48
1:A:50:VAL:HG22	1:B:288:VAL:HG11	1.96	0.48
1:C:57:GLU:HA	1:C:57:GLU:OE1	2.13	0.48
1:A:279:MET:O	1:A:284:LEU:HB2	2.14	0.48
1:B:152:ILE:HG22	1:B:156:LEU:HD22	1.96	0.48
1:D:120:LEU:HB2	1:D:169:PHE:HB3	1.96	0.48
1:D:167:MET:O	1:D:170:ILE:HG22	2.14	0.48
1:D:237:ASN:ND2	1:D:237:ASN:C	2.67	0.48
1:A:92:VAL:HG23	1:A:208:PHE:CE1	2.49	0.48
1:C:100:ASP:OD1	1:C:105:TYR:CD2	2.67	0.48
1:D:289:ASN:O	1:D:292:VAL:HG22	2.14	0.48
1:A:203:ARG:HB2	1:A:280:HIS:HB3	1.96	0.47
1:A:217:VAL:C	1:A:221:THR:HG22	2.35	0.47
1:B:99:PHE:HE1	1:B:121:PHE:CD1	2.32	0.47
1:A:103:SER:C	1:A:105:TYR:H	2.18	0.47
1:A:213:GLU:O	1:A:216:ALA:N	2.48	0.47
1:B:151:TRP:CD1	1:B:289:ASN:HB2	2.49	0.47
1:B:165:HIS:CD2	1:B:262:ILE:HD13	2.49	0.47
1:B:177:LEU:N	1:B:178:PRO:HD2	2.29	0.47
1:D:144:TYR:O	1:D:145:MET:C	2.51	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:266:GLU:OE2	1:D:266:GLU:HA	2.14	0.47
1:A:142:LEU:HD23	1:B:166:LEU:HD12	1.95	0.47
1:D:209:VAL:O	1:D:210:GLY:C	2.50	0.47
1:B:153:ASN:O	1:B:157:VAL:HG13	2.13	0.47
1:C:221:THR:HB	1:C:263:ARG:HE	1.80	0.47
1:C:92:VAL:HG22	1:C:208:PHE:CE1	2.49	0.47
1:C:109:SER:O	1:C:111:THR:N	2.39	0.47
1:C:144:TYR:CD2	1:C:144:TYR:N	2.82	0.47
1:D:261:VAL:O	1:D:263:ARG:N	2.48	0.47
1:A:187:GLN:NE2	1:B:143:ARG:NH1	2.54	0.47
1:A:245:VAL:CG2	1:A:246:TYR:N	2.77	0.47
1:B:55:SER:O	1:B:62:ARG:NH2	2.48	0.47
1:A:270:ARG:O	1:A:271:VAL:C	2.53	0.47
1:A:41:LEU:HD22	1:B:78:LYS:CB	2.46	0.46
1:D:205:VAL:O	1:D:209:VAL:HG23	2.15	0.46
1:A:294:LEU:HD12	1:A:294:LEU:HA	1.73	0.46
1:B:289:ASN:O	1:B:292:VAL:HG22	2.15	0.46
1:C:66:SER:O	1:C:70:ILE:HG12	2.16	0.46
1:A:102:PHE:CD1	1:A:102:PHE:N	2.83	0.46
1:C:217:VAL:O	1:C:221:THR:CG2	2.55	0.46
1:C:63:PRO:HG2	1:C:247:TRP:CD1	2.51	0.46
1:C:177:LEU:O	1:C:181:VAL:HG23	2.16	0.46
1:C:231:ARG:HH21	1:C:231:ARG:CB	2.28	0.46
1:A:100:ASP:OD1	1:A:118:ARG:NH2	2.43	0.46
1:B:263:ARG:O	1:B:263:ARG:HG2	2.15	0.46
1:D:207:ARG:HH11	1:D:274:HIS:HD2	1.63	0.46
1:C:216:ALA:O	1:C:219:THR:HB	2.15	0.46
1:A:40:ARG:HG2	1:D:72:ASN:HD21	1.80	0.46
1:D:163:ARG:O	1:D:166:LEU:HB3	2.15	0.46
1:D:273:ASN:O	1:D:274:HIS:C	2.54	0.46
1:A:161:ASN:HA	1:A:246:TYR:OH	2.17	0.46
1:A:206:HIS:ND1	1:A:273:ASN:ND2	2.64	0.46
1:C:231:ARG:O	1:C:233:ARG:NH2	2.48	0.46
1:B:207:ARG:CZ	1:B:277:ALA:HB3	2.46	0.45
1:B:215:GLU:O	1:B:216:ALA:C	2.55	0.45
1:D:142:LEU:O	1:D:143:ARG:C	2.55	0.45
1:D:291:PHE:HA	1:D:294:LEU:HB2	1.99	0.45
1:A:151:TRP:CD1	1:A:289:ASN:HB2	2.51	0.45
1:A:163:ARG:O	1:A:167:MET:HG2	2.17	0.45
1:A:280:HIS:CG	1:A:285:GLN:HG3	2.51	0.45
1:B:144:TYR:O	1:B:145:MET:C	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:LYS:O	1:C:211:TYR:HE1	1.99	0.45
1:D:236:LYS:C	1:D:238:ASP:H	2.20	0.45
1:B:128:VAL:H	1:B:129:PRO:HD2	1.81	0.45
1:B:241:GLU:O	1:B:244:ARG:HB2	2.17	0.45
1:B:169:PHE:HA	1:B:172:LEU:HD12	1.99	0.45
1:C:257:ASP:CG	4:C:603:HOH:O	2.54	0.45
1:B:267:ALA:HA	1:B:270:ARG:HB3	1.98	0.45
1:C:185:ILE:HD12	1:C:189:ILE:HD11	1.99	0.45
1:C:249:LEU:HD22	1:C:253:ALA:CB	2.47	0.45
1:A:110:ILE:O	1:A:110:ILE:CG2	2.65	0.45
1:A:267:ALA:O	1:A:270:ARG:HB3	2.17	0.45
1:D:118:ARG:HH21	1:D:219:THR:CG2	2.29	0.45
1:D:220:TYR:CE2	1:D:266:GLU:HG3	2.52	0.45
1:A:218:ILE:HA	1:A:221:THR:HG22	1.99	0.44
1:B:89:TYR:HD1	1:B:211:TYR:CG	2.35	0.44
1:C:291:PHE:O	1:C:295:LYS:HG3	2.17	0.44
1:D:258:LEU:C	1:D:258:LEU:CD2	2.85	0.44
1:A:225:ARG:HD2	1:C:77:HIS:CE1	2.53	0.44
1:D:131:MET:O	1:D:135:MET:HB2	2.17	0.44
1:B:132:VAL:O	1:B:133:GLY:C	2.56	0.44
1:C:212:LEU:HD23	1:C:212:LEU:HA	1.49	0.44
1:C:257:ASP:O	1:C:261:VAL:HG22	2.18	0.44
1:A:46:THR:HA	1:A:49:VAL:HG22	1.99	0.44
1:A:169:PHE:C	1:A:171:GLU:H	2.21	0.44
1:D:236:LYS:O	1:D:238:ASP:N	2.51	0.44
1:A:272:VAL:HA	1:A:291:PHE:CZ	2.52	0.44
1:B:70:ILE:HG13	1:B:71:GLU:N	2.30	0.44
1:B:96:ARG:HH22	1:B:219:THR:HG1	1.62	0.44
1:C:177:LEU:HB2	1:C:178:PRO:HD3	1.99	0.44
1:D:218:ILE:O	1:D:219:THR:C	2.55	0.44
1:A:97:TRP:O	1:A:101:THR:HG23	2.16	0.44
1:B:207:ARG:CZ	1:B:277:ALA:CB	2.96	0.44
1:A:218:ILE:O	1:A:219:THR:C	2.57	0.43
1:C:75:ILE:HD13	1:C:218:ILE:HG12	2.00	0.43
1:C:112:GLU:O	1:C:113:SER:C	2.56	0.43
1:C:123:GLU:HA	1:C:126:ALA:HB3	2.00	0.43
1:D:111:THR:HG22	1:D:113:SER:HB2	1.99	0.43
1:D:137:ARG:NH1	1:D:151:TRP:CD2	2.87	0.43
1:A:104:LEU:C	1:A:106:ARG:N	2.71	0.43
1:A:209:VAL:CG1	1:A:273:ASN:OD1	2.66	0.43
1:B:160:GLU:O	1:B:163:ARG:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:MET:HE1	1:B:147:ARG:N	2.33	0.43
1:B:85:ASP:OD2	1:B:207:ARG:NE	2.51	0.43
1:A:207:ARG:O	1:A:208:PHE:C	2.57	0.43
1:C:89:TYR:CE1	1:C:93:ARG:HG3	2.54	0.43
1:D:158:GLU:OE1	1:D:269:HIS:HD2	2.02	0.43
1:D:261:VAL:C	1:D:263:ARG:N	2.70	0.43
1:C:272:VAL:HA	1:C:291:PHE:CE2	2.54	0.43
1:B:99:PHE:CE1	1:B:121:PHE:CD1	3.07	0.42
1:B:160:GLU:O	1:B:161:ASN:C	2.56	0.42
1:A:77:HIS:CG	1:C:225:ARG:NE	2.87	0.42
1:C:47:VAL:HG13	1:C:48:PRO:HD3	2.01	0.42
1:D:35:HIS:HD2	1:D:39:ASN:HD22	1.68	0.42
1:D:207:ARG:NH2	1:D:278:ASP:OD1	2.49	0.42
1:D:209:VAL:HB	1:D:273:ASN:ND2	2.34	0.42
1:A:101:THR:HG22	4:A:603:HOH:O	2.19	0.42
1:C:118:ARG:O	1:C:118:ARG:HG2	2.17	0.42
1:C:138:HIS:HA	1:C:152:ILE:CD1	2.49	0.42
1:D:47:VAL:HG22	1:D:48:PRO:HD3	2.00	0.42
1:B:65:TRP:HB3	1:B:70:ILE:HG21	2.02	0.42
1:C:207:ARG:HG3	1:C:211:TYR:CE2	2.55	0.42
1:D:44:LEU:O	1:D:47:VAL:HG13	2.20	0.42
1:A:234:PRO:C	1:A:237:ASN:HD21	2.23	0.42
1:B:280:HIS:O	1:B:282:LYS:N	2.52	0.42
1:C:43:PHE:O	1:C:45:GLU:N	2.53	0.42
1:D:272:VAL:CG1	1:D:273:ASN:N	2.81	0.42
1:C:276:PHE:O	1:C:277:ALA:C	2.57	0.42
1:D:111:THR:HB	1:D:114:LYS:HG2	2.02	0.42
1:B:54:VAL:HB	1:B:241:GLU:OE1	2.19	0.42
1:B:270:ARG:O	1:B:274:HIS:HB2	2.20	0.42
1:D:258:LEU:O	1:D:261:VAL:HG23	2.19	0.42
1:A:106:ARG:HB3	4:A:608:HOH:O	2.19	0.42
1:A:273:ASN:HD22	1:A:273:ASN:HA	1.63	0.42
1:B:53:ARG:O	1:B:55:SER:N	2.53	0.42
1:B:70:ILE:HD12	1:B:264:ALA:HB2	2.02	0.42
1:B:73:VAL:HB	1:B:263:ARG:HH11	1.83	0.42
1:D:93:ARG:NH2	1:D:96:ARG:HH11	2.18	0.42
1:A:96:ARG:NH1	1:A:118:ARG:HH21	2.17	0.41
1:C:111:THR:O	1:C:112:GLU:C	2.58	0.41
1:A:138:HIS:NE2	1:B:127:GLY:O	2.51	0.41
1:B:106:ARG:H	1:B:106:ARG:HG3	1.72	0.41
1:B:114:LYS:HB3	1:B:114:LYS:HE2	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ASN:O	1:A:73:VAL:C	2.58	0.41
1:A:168:THR:HG23	1:A:243:ALA:HB2	2.02	0.41
1:B:220:TYR:CB	1:B:263:ARG:HB2	2.50	0.41
1:B:223:VAL:HG12	1:B:227:ILE:HD12	2.02	0.41
1:B:41:LEU:HG	1:C:72:ASN:CG	2.41	0.41
1:B:88:ALA:O	1:B:92:VAL:HG23	2.20	0.41
1:C:218:ILE:HA	1:C:221:THR:HG23	2.01	0.41
1:D:53:ARG:O	1:D:56:ASP:HB2	2.21	0.41
1:A:293:VAL:HG12	1:A:294:LEU:N	2.34	0.41
1:B:84:VAL:HB	1:B:203:ARG:HH21	1.85	0.41
1:A:49:VAL:O	1:B:299:GLU:HG2	2.21	0.41
1:B:296:LYS:HG3	1:B:297:ASN:H	1.82	0.41
1:C:128:VAL:N	1:C:129:PRO:CD	2.84	0.41
1:A:135:MET:HE1	1:B:135:MET:HE3	2.03	0.41
1:C:194:LEU:HA	1:C:197:ALA:HB3	2.02	0.41
1:A:57:GLU:O	1:A:163:ARG:NH1	2.54	0.41
1:A:251:LYS:H	1:A:251:LYS:HG2	1.49	0.41
1:B:44:LEU:C	1:B:44:LEU:HD22	2.41	0.41
1:B:69:ASP:OD1	1:B:69:ASP:C	2.59	0.41
1:C:37:GLN:CD	1:C:37:GLN:N	2.74	0.41
1:D:152:ILE:HG22	1:D:156:LEU:HD22	2.02	0.41
1:D:158:GLU:HG3	1:D:269:HIS:CD2	2.56	0.41
1:D:251:LYS:H	1:D:251:LYS:HG2	1.66	0.41
1:A:166:LEU:HD12	1:B:142:LEU:HA	2.01	0.41
1:B:224:MET:CE	1:B:260:ASN:HD22	2.34	0.41
1:B:293:VAL:HG11	1:B:299:GLU:HG3	2.02	0.41
1:D:168:THR:HG23	1:D:240:PRO:HG2	2.00	0.41
1:A:104:LEU:O	1:A:106:ARG:N	2.53	0.40
1:B:239:VAL:CG2	1:B:258:LEU:HD12	2.48	0.40
1:D:137:ARG:CZ	1:D:151:TRP:CG	3.05	0.40
1:D:138:HIS:O	1:D:141:SER:OG	2.35	0.40
1:D:216:ALA:O	1:D:220:TYR:CD2	2.74	0.40
1:A:297:ASN:N	1:A:297:ASN:ND2	2.68	0.40
1:D:218:ILE:HG22	1:D:219:THR:N	2.35	0.40
1:D:220:TYR:HB2	1:D:263:ARG:HB2	2.03	0.40
1:A:80:PRO:HG3	1:C:228:ASP:HB3	2.03	0.40
1:A:143:ARG:HA	1:B:183:ILE:CG2	2.51	0.40
1:C:227:ILE:O	1:C:228:ASP:C	2.59	0.40
1:C:289:ASN:OD1	1:C:290:PRO:HD2	2.21	0.40
1:D:158:GLU:OE1	1:D:269:HIS:CD2	2.75	0.40
1:A:209:VAL:O	1:A:210:GLY:C	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:ALA:O	1:C:160:GLU:C	2.59	0.40
1:D:109:SER:OG	1:D:231:ARG:NH1	2.53	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	265/329 (80%)	203 (77%)	48 (18%)	14 (5%)	2 5
1	B	266/329 (81%)	208 (78%)	50 (19%)	8 (3%)	4 14
1	C	264/329 (80%)	201 (76%)	48 (18%)	15 (6%)	1 4
1	D	264/329 (80%)	206 (78%)	44 (17%)	14 (5%)	2 5
All	All	1059/1316 (80%)	818 (77%)	190 (18%)	51 (5%)	2 6

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	71	GLU
1	B	297	ASN
1	C	110	ILE
1	D	103	SER
1	A	105	TYR
1	A	270	ARG
1	A	271	VAL
1	B	281	GLU
1	B	283	ARG
1	C	44	LEU
1	C	89	TYR
1	C	113	SER
1	C	182	SER

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Mol	Chain	Res	Type
1	D	104	LEU
1	D	218	ILE
1	D	237	ASN
1	A	112	GLU
1	A	165	HIS
1	A	219	THR
1	A	248	ASN
1	C	181	VAL
1	C	238	ASP
1	C	296	LYS
1	D	112	GLU
1	D	120	LEU
1	D	234	PRO
1	A	113	SER
1	A	156	LEU
1	A	265	ASP
1	B	106	ARG
1	B	110	ILE
1	C	80	PRO
1	C	283	ARG
1	D	106	ARG
1	D	128	VAL
1	D	145	MET
1	D	262	ILE
1	A	140	SER
1	A	167	MET
1	B	190	MET
1	D	200	ILE
1	A	152	ILE
1	C	129	PRO
1	D	183	ILE
1	C	223	VAL
1	A	170	ILE
1	D	217	VAL
1	B	54	VAL
1	C	73	VAL
1	C	259	ILE
1	C	210	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	242/292 (83%)	206 (85%)	36 (15%)	3 8
1	B	243/292 (83%)	208 (86%)	35 (14%)	3 8
1	C	241/292 (82%)	192 (80%)	49 (20%)	1 3
1	D	241/292 (82%)	204 (85%)	37 (15%)	2 7
All	All	967/1168 (83%)	810 (84%)	157 (16%)	2 6

All (157) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	THR
1	A	44	LEU
1	A	45	GLU
1	A	50	VAL
1	A	52	LEU
1	A	54	VAL
1	A	66	SER
1	A	87	LEU
1	A	94	THR
1	A	98	LEU
1	A	106	ARG
1	A	109	SER
1	A	110	ILE
1	A	111	THR
1	A	116	ILE
1	A	125	VAL
1	A	132	VAL
1	A	135	MET
1	A	136	LEU
1	A	158	GLU
1	A	166	LEU
1	A	170	ILE
1	A	185	ILE
1	A	231	ARG

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Mol	Chain	Res	Type
1	A	232	LEU
1	A	233	ARG
1	A	235	THR
1	A	238	ASP
1	A	242	VAL
1	A	245	VAL
1	A	254	THR
1	A	258	LEU
1	A	271	VAL
1	A	284	LEU
1	A	285	GLN
1	A	297	ASN
1	B	40	ARG
1	B	44	LEU
1	B	46	THR
1	B	47	VAL
1	B	50	VAL
1	B	54	VAL
1	B	60	GLU
1	B	64	THR
1	B	87	LEU
1	B	96	ARG
1	B	98	LEU
1	B	106	ARG
1	B	110	ILE
1	B	111	THR
1	B	136	LEU
1	B	143	ARG
1	B	156	LEU
1	B	166	LEU
1	B	170	ILE
1	B	171	GLU
1	B	174	GLN
1	B	177	LEU
1	B	184	ILE
1	B	212	LEU
1	B	221	THR
1	B	225	ARG
1	B	242	VAL
1	B	248	ASN
1	B	251	LYS
1	B	258	LEU

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Mol	Chain	Res	Type
1	B	261	VAL
1	B	262	ILE
1	B	263	ARG
1	B	274	HIS
1	B	284	LEU
1	C	32	VAL
1	C	33	TRP
1	C	44	LEU
1	C	47	VAL
1	C	52	LEU
1	C	54	VAL
1	C	64	THR
1	C	72	ASN
1	C	83	LEU
1	C	84	VAL
1	C	86	THR
1	C	87	LEU
1	C	89	TYR
1	C	91	SER
1	C	96	ARG
1	C	102	PHE
1	C	103	SER
1	C	104	LEU
1	C	110	ILE
1	C	114	LYS
1	C	115	VAL
1	C	118	ARG
1	C	119	CYS
1	C	124	THR
1	C	132	VAL
1	C	136	LEU
1	C	140	SER
1	C	146	THR
1	C	147	ARG
1	C	156	LEU
1	C	157	VAL
1	C	170	ILE
1	C	179	LEU
1	C	185	ILE
1	C	194	LEU
1	C	212	LEU
1	C	221	THR

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Mol	Chain	Res	Type
1	C	225	ARG
1	C	231	ARG
1	C	233	ARG
1	C	238	ASP
1	C	248	ASN
1	C	254	THR
1	C	257	ASP
1	C	258	LEU
1	C	261	VAL
1	C	274	HIS
1	C	285	GLN
1	C	288	VAL
1	D	35	HIS
1	D	44	LEU
1	D	50	VAL
1	D	66	SER
1	D	73	VAL
1	D	81	ASN
1	D	83	LEU
1	D	85	ASP
1	D	91	SER
1	D	94	THR
1	D	100	ASP
1	D	118	ARG
1	D	123	GLU
1	D	132	VAL
1	D	153	ASN
1	D	156	LEU
1	D	170	ILE
1	D	179	LEU
1	D	182	SER
1	D	192	LEU
1	D	221	THR
1	D	232	LEU
1	D	233	ARG
1	D	237	ASN
1	D	238	ASP
1	D	242	VAL
1	D	245	VAL
1	D	250	SER
1	D	251	LYS
1	D	258	LEU

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Mol	Chain	Res	Type
1	D	260	ASN
1	D	263	ARG
1	D	271	VAL
1	D	272	VAL
1	D	284	LEU
1	D	292	VAL
1	D	295	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	161	ASN
1	A	187	GLN
1	A	237	ASN
1	A	248	ASN
1	A	269	HIS
1	A	273	ASN
1	A	285	GLN
1	A	297	ASN
1	B	174	GLN
1	B	187	GLN
1	B	206	HIS
1	B	237	ASN
1	B	248	ASN
1	B	260	ASN
1	B	273	ASN
1	B	274	HIS
1	B	280	HIS
1	B	285	GLN
1	C	77	HIS
1	C	165	HIS
1	C	248	ASN
1	C	260	ASN
1	C	269	HIS
1	C	273	ASN
1	C	274	HIS
1	C	285	GLN
1	D	35	HIS
1	D	72	ASN
1	D	237	ASN
1	D	269	HIS

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Mol	Chain	Res	Type
1	D	274	HIS
1	D	285	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 8 are monoatomic and 4 are modelled with single atom - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	267/329 (81%)	-0.10	4 (1%)	73	72	54, 76, 104, 132	0
1	B	268/329 (81%)	-0.10	12 (4%)	33	28	53, 75, 108, 152	0
1	C	266/329 (80%)	0.09	11 (4%)	37	31	61, 90, 137, 175	0
1	D	266/329 (80%)	0.05	13 (4%)	29	25	54, 81, 123, 157	0
All	All	1067/1316 (81%)	-0.02	40 (3%)	41	36	53, 80, 119, 175	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	109	SER	5.9
1	C	110	ILE	4.7
1	C	235	THR	4.5
1	A	52	LEU	4.5
1	C	175	PRO	4.0
1	B	49	VAL	3.8
1	B	253	ALA	3.7
1	B	236	LYS	3.6
1	B	48	PRO	3.3
1	D	109	SER	3.2
1	D	99	PHE	3.1
1	D	106	ARG	3.1
1	C	97	TRP	3.0
1	A	49	VAL	3.0
1	B	297	ASN	2.9
1	D	51	PRO	2.9
1	D	110	ILE	2.9
1	B	47	VAL	2.8
1	C	251	LYS	2.8
1	D	105	TYR	2.8
1	C	66	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	107	PHE	2.6
1	C	33	TRP	2.6
1	D	111	THR	2.5
1	D	98	LEU	2.5
1	B	283	ARG	2.4
1	A	276	PHE	2.4
1	D	252	ASN	2.4
1	D	113	SER	2.4
1	C	102	PHE	2.3
1	B	238	ASP	2.3
1	B	237	ASN	2.3
1	D	245	VAL	2.3
1	C	54	VAL	2.2
1	B	258	LEU	2.2
1	A	253	ALA	2.1
1	B	235	THR	2.1
1	D	52	LEU	2.1
1	B	254	THR	2.0
1	C	249	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FE	B	501	1/1	0.85	0.18	78,78,78,78	0
2	FE	A	502	1/1	0.89	0.19	70,70,70,70	0
2	FE	B	502	1/1	0.90	0.17	64,64,64,64	0
2	FE	A	501	1/1	0.92	0.10	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FE	C	502	1/1	0.93	0.21	71,71,71,71	0
3	OH	A	503	1/1	0.95	0.15	43,43,43,43	0
2	FE	D	502	1/1	0.96	0.17	59,59,59,59	0
2	FE	D	501	1/1	0.97	0.20	84,84,84,84	0
3	OH	B	503	1/1	0.97	0.38	40,40,40,40	0
2	FE	C	501	1/1	0.99	0.18	79,79,79,79	0
3	OH	C	503	1/1	0.99	0.28	36,36,36,36	0
3	OH	D	503	1/1	0.99	0.31	79,79,79,79	0

6.5 Other polymers (i)

There are no such residues in this entry.