Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:43 AM GMT

PDB ID	:	2E3T
Title	:	Crystal structure of rat xanthine oxidoreductase mutant (W335A and F336L)
Authors	:	Asai, R.; Nishino, T.; Matsumura, T.; Okamoto, K.; Pai, E.F.; Nishino, T.
Deposited on	:	2006-11-28
Resolution	:	2.28 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:

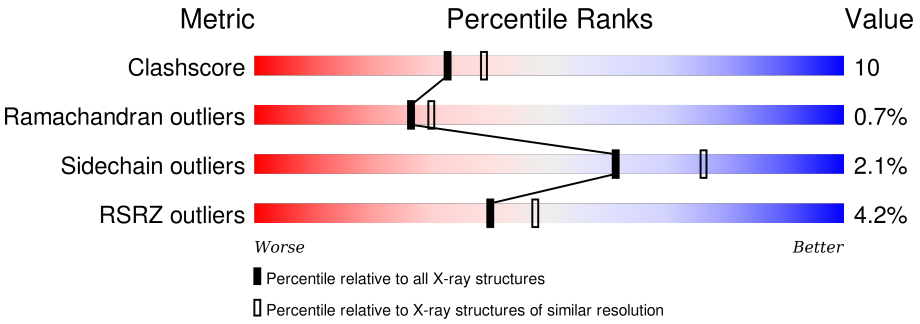
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.28 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))
Clashscore	102246	5929 (2.30-2.26)
Ramachandran outliers	100387	5851 (2.30-2.26)
Sidechain outliers	100360	5850 (2.30-2.26)
RSRZ outliers	91569	5204 (2.30-2.26)

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	1331	5% 77% 18%
1	B	1331	3% 78% 18%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	A	6006	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 21444 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.

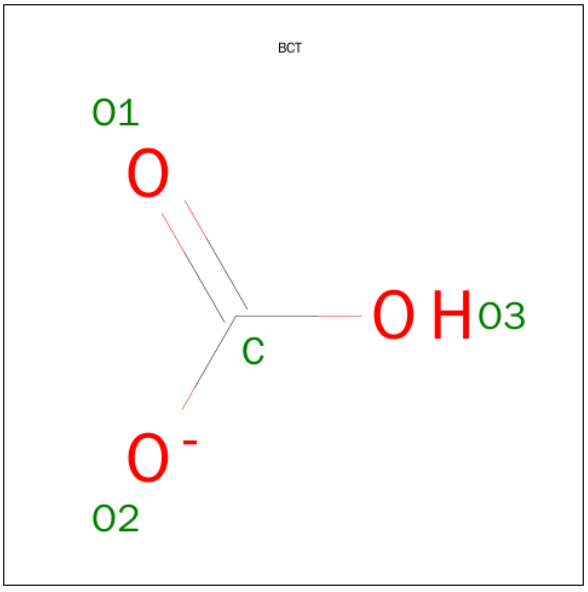
- Molecule 1 is a protein called Xanthine dehydrogenase/oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1291	Total	C	N	O	S	0	0	0
			9963	6309	1715	1875	64			
1	B	1281	Total	C	N	O	S	0	0	0
			9877	6255	1702	1858	62			

There are 4 discrepancies between the modelled and reference sequences:

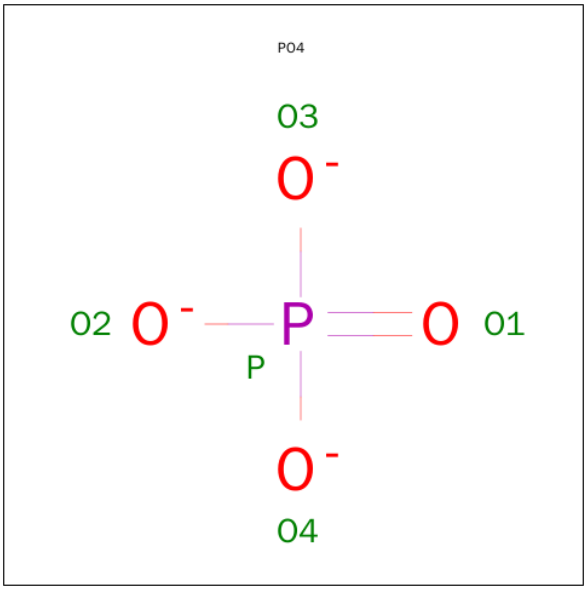
Chain	Residue	Modelled	Actual	Comment	Reference
A	335	ALA	TRP	ENGINEERED	UNP P22985
A	336	LEU	PHE	ENGINEERED	UNP P22985
B	335	ALA	TRP	ENGINEERED	UNP P22985
B	336	LEU	PHE	ENGINEERED	UNP P22985

- Molecule 2 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 1 3	0	0
2	B	1	Total C O 4 1 3	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0

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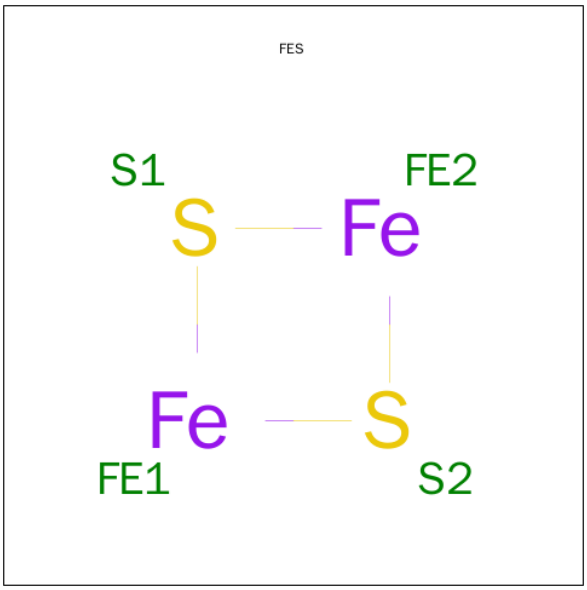
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O P 5 4 1	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

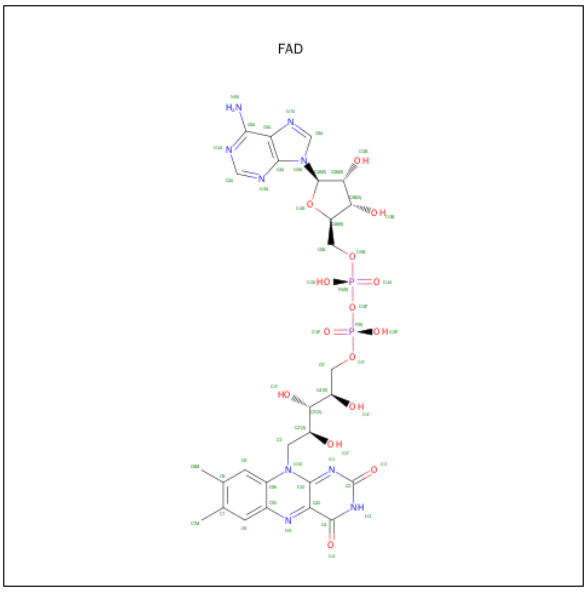
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	2	Total Ca 2 2	0	0
4	A	2	Total Ca 2 2	0	0

- Molecule 5 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



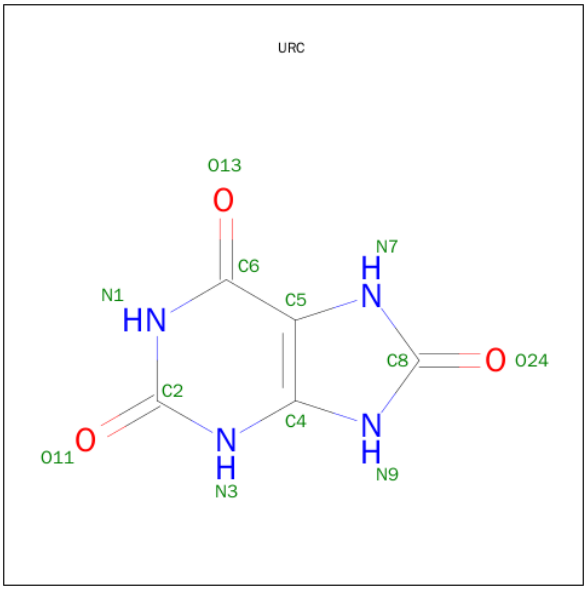
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Fe S 4 2 2	0	0
5	A	1	Total Fe S 4 2 2	0	0
5	B	1	Total Fe S 4 2 2	0	0
5	B	1	Total Fe S 4 2 2	0	0

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
6	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 7 is URIC ACID (three-letter code: URC) (formula: $C_5H_4N_4O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			12	5	4	3		
7	B	1	Total	C	N	O	0	0
			12	5	4	3		

- Molecule 8 is water.

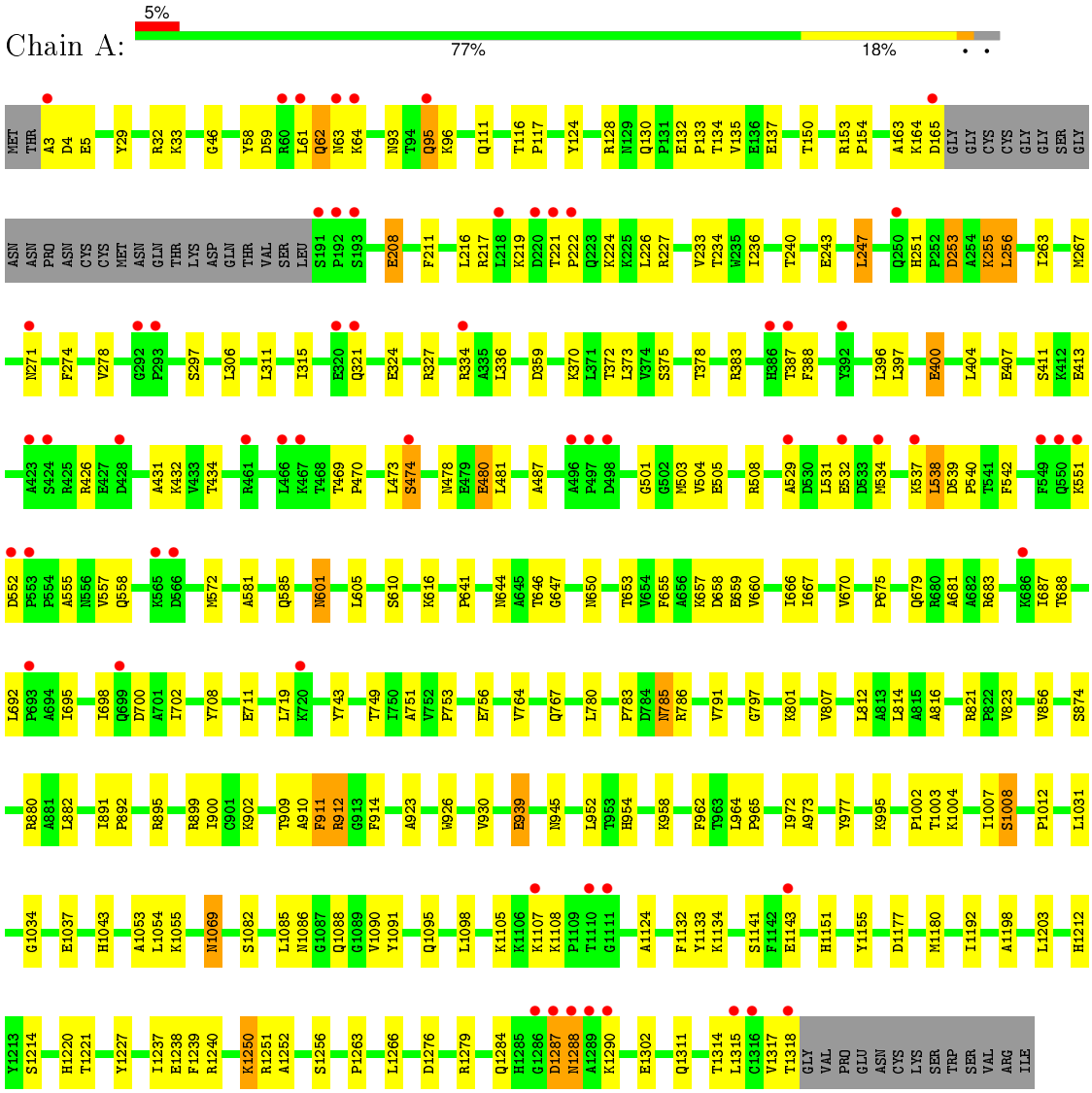
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	667	Total O 667 667	0	0
8	B	724	Total O 724 724	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

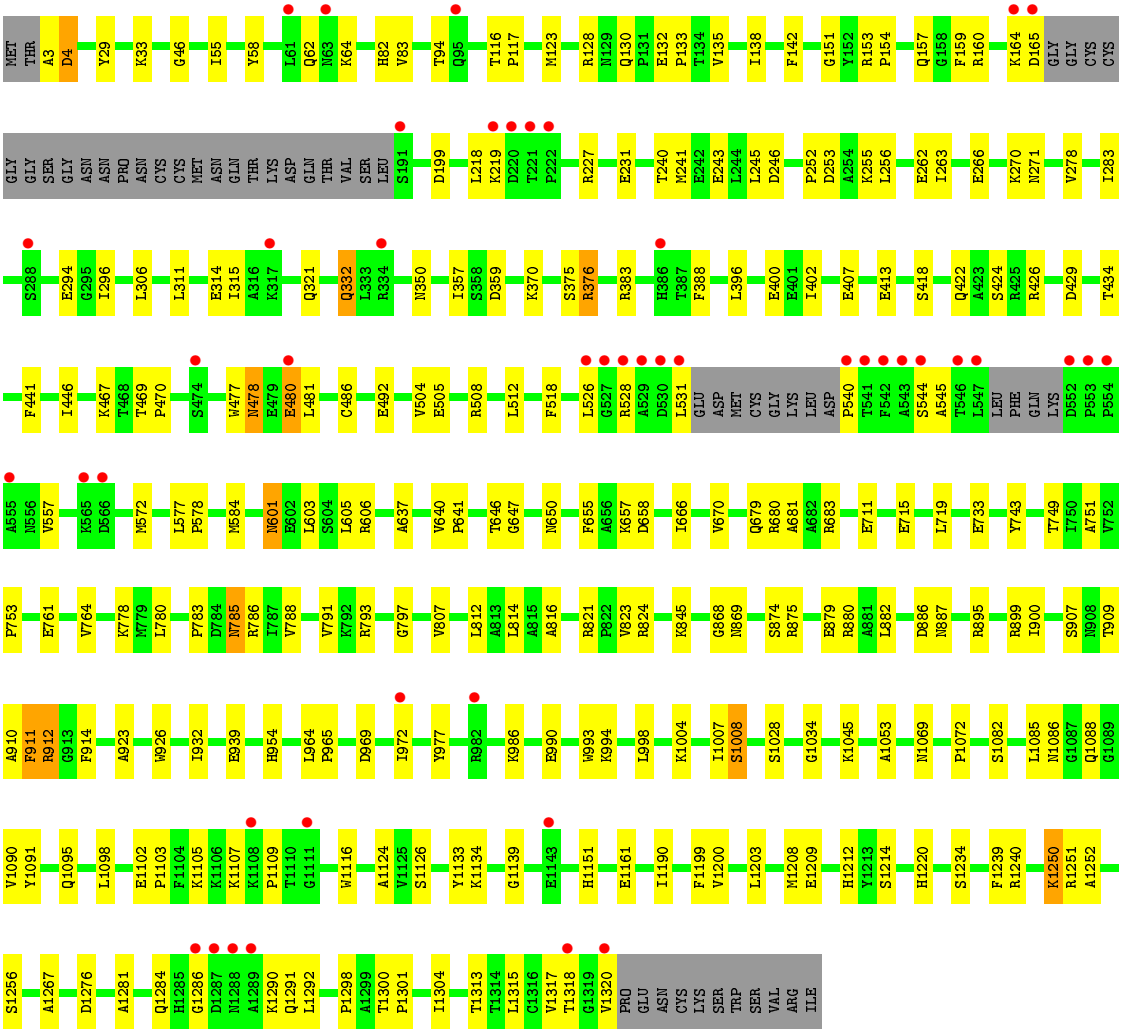
- Molecule 1: Xanthine dehydrogenase/oxidase

Chain A:



- Molecule 1: Xanthine dehydrogenase/oxidase

Chain B:


MET THR A3 D4 Y29 K33 G46 I55 Y58 L61 Q62 N63 K64 H82 V83 T94 Q95 T116 P117 M123 R128 N129 Q130 P131 E132 P133 T134 V135 I138 F142 G151 Y152 R153 P154 Q157 G158 F159 R160 K164 D165 GLY GLY CYS CYS
GLY GLY SER GLY ASN ASN PRO ASN CYS CYS MET ASN GLN THR LYS ASP GLN THR VAL SER LEU S191 D199 L218 K219 D220 T221 P222 R227 E231 T240 M241 E242 E243 L244 L245 D246 P252 D253 A254 K255 L256 E262 I263 E266 K270 N271 V278 I283
S288 E294 G295 I296 L306 L311 E314 I315 A316 K317 Q321 Q332 L333 R334 N350 I357 S358 D359 K370 S375 R376 R383 H386 T387 F388 L396 E400 E401 I402 E407 E413 S418 Q422 A423 S424 R425 R426 D429 T434
F441 I446 K467 T468 T469 P470 S474 W477 N478 E479 E480 L481 C486 E492 V504 E505 R508 L512 F518 L526 G527 R528 A529 D530 L531 GLU ASP MET CYS GLY LYS LEU ASP P540 T541 F542 A543 S544 A545 T546 L547 LEU PHE GLN LYS D552 P553 P554
A555 N556 V557 K565 D566 M572 L577 P578 M584 N601 E602 L603 S604 L605 R606 A637 V640 P641 T646 G647 N650 F655 A656 K657 D658 I666 V670 Q679 R680 A681 A682 R683 E711 E715 L719 E733 Y743 T749 I750 A751 V752
P753 E761 V764 K778 M779 L780 P783 D784 N785 R786 I787 V788 V791 K792 R793 G797 V807 L812 A813 L814 A815 A816 R821 P822 V823 R824 K845 G868 N869 S874 R875 E879 R880 A881 L882 D886 N887 R895 R899 I900 S907 N908 T909
A910 F911 R912 G913 F914 A923 W926 I932 E939 H954 L964 P965 D969 I972 Y977 R982 K986 E990 W993 K994 L998 K1004 I1007 S1008 S1028 G1034 K1045 A1053 N1069 P1072 S1082 L1085 N1086 G1087 Q1088 G1089
V1090 Y1091 Q1095 L1098 E1102 P1103 F1104 K1105 K1106 K1107 K1108 P1109 T1110 G1111 W1116 A1124 V1125 S1126 Y1133 K1134 G1139 E1143 H1151 E1161 I1190 F1199 V1200 L1203 M1208 E1209 H1212 Y1213 S1214 H1220 S1234 F1239 R1240 K1250 R1251 A1252
S1256 A1267 D1276 A1281 Q1284 H1285 G1286 D1287 N1288 A1289 K1290 Q1291 L1292 P1298 A1299 T1300 P1301 I1304 T1313 T1314 L1315 C1316 V1317 T1318 G1319 V1320 PRO GLU ASN CYS LYS SER TRP SER VAL ARG ILE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	101.07Å 139.51Å 222.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.28 24.94 – 2.28	Depositor EDS
% Data completeness (in resolution range)	100.0 (25.00-2.28) 95.8 (24.94-2.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	5.84 (at 2.28Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.185 , 0.229 0.181 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	27.2	Xtriage
Anisotropy	0.538	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 47.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 143383 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	21444	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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: URC, PO4, FES, BCT, CA, FAD

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	0.32	0/10170	0.60	0/13763
1	B	0.33	0/10081	0.61	0/13642
All	All	0.33	0/20251	0.60	0/27405

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	9963	0	9972	208	0
1	B	9877	0	9888	211	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
3	A	30	0	0	1	0
3	B	25	0	0	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	8	0	0	1	0
5	B	8	0	0	1	0
6	A	53	0	28	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	53	0	26	3	0
7	A	12	0	4	0	0
7	B	12	0	4	0	0
8	A	667	0	0	7	0
8	B	724	0	0	7	0
All	All	21444	0	19922	415	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 10.

All (415) 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)
6:B:3003:FAD:C3B	6:B:3003:FAD:C2B	1.79	1.41
1:B:3:ALA:HB1	1:B:227:ARG:H	1.16	1.05
1:A:3:ALA:HB1	1:A:227:ARG:H	1.24	1.01
1:B:646:THR:HG22	1:B:647:GLY:H	1.28	0.97
1:A:646:THR:HG22	1:A:647:GLY:H	1.30	0.95
1:B:359:ASP:HA	1:B:434:THR:HG21	1.54	0.89
1:B:3:ALA:HB1	1:B:227:ARG:N	1.86	0.89
1:B:130:GLN:HE21	1:B:132:GLU:H	1.16	0.88
1:B:785:ASN:HD21	1:B:786:ARG:NH1	1.73	0.86
1:B:252:PRO:HG3	1:B:400:GLU:HG2	1.58	0.85
1:A:785:ASN:HD21	1:A:786:ARG:HH11	1.24	0.85
1:B:1088:GLN:HG2	1:B:1133:TYR:CD1	2.13	0.84
1:B:785:ASN:HD21	1:B:786:ARG:HH11	1.21	0.84
1:A:1088:GLN:HG2	1:A:1133:TYR:CD1	2.12	0.83
1:A:359:ASP:HA	1:A:434:THR:HG21	1.58	0.83
1:A:3:ALA:N	1:A:224:LYS:HZ2	1.77	0.81
1:A:130:GLN:HE21	1:A:132:GLU:H	1.29	0.81
1:A:555:ALA:HB3	1:A:1238:GLU:HG3	1.62	0.80
1:A:749:THR:HG22	1:A:812:LEU:HD23	1.63	0.80
1:A:939:GLU:HG2	1:A:977:TYR:CE2	2.17	0.79
1:A:557:VAL:HG12	1:A:1240:ARG:HG2	1.65	0.78
1:A:785:ASN:HD21	1:A:786:ARG:NH1	1.82	0.77
1:B:321:GLN:HG2	1:B:413:GLU:OE2	1.85	0.77
1:B:932:ILE:O	1:B:1290:LYS:HE3	1.84	0.76
1:B:785:ASN:ND2	1:B:786:ARG:HH11	1.82	0.76
1:B:650:ASN:HD21	1:B:778:LYS:NZ	1.83	0.76
1:A:1141:SER:OG	1:A:1143:GLU:HG2	1.87	0.75
1:B:332:GLN:HE21	1:B:332:GLN:HA	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:785:ASN:ND2	1:A:786:ARG:HH11	1.86	0.74
1:B:719:LEU:HD11	1:B:895:ARG:HB3	1.70	0.74
1:A:388:PHE:HA	1:A:396:LEU:HG	1.71	0.72
1:B:58:TYR:CE2	1:B:219:LYS:HG3	2.24	0.72
1:B:531:LEU:HA	1:B:540:PRO:HD2	1.73	0.71
1:B:749:THR:HG22	1:B:812:LEU:HD23	1.72	0.71
1:B:749:THR:HG22	1:B:812:LEU:CD2	2.20	0.71
1:B:939:GLU:HG2	1:B:977:TYR:CE2	2.24	0.71
1:B:1102:GLU:HB3	1:B:1103:PRO:HD3	1.72	0.71
1:A:749:THR:HG22	1:A:812:LEU:CD2	2.20	0.70
1:A:487:ALA:HA	1:A:1318:THR:HG23	1.73	0.69
1:A:3:ALA:HB1	1:A:227:ARG:N	2.05	0.69
1:B:1315:LEU:HA	1:B:1320:VAL:O	1.92	0.69
1:A:719:LEU:HD11	1:A:895:ARG:HB2	1.75	0.69
1:A:537:LYS:O	1:A:538:LEU:HB3	1.93	0.67
1:A:61:LEU:O	1:A:62:GLN:HG3	1.94	0.67
1:A:1124:ALA:HB3	1:B:1134:LYS:HD3	1.77	0.67
1:B:1290:LYS:O	1:B:1290:LYS:HG2	1.94	0.66
1:A:375:SER:HB3	1:A:378:THR:OG1	1.95	0.66
1:B:650:ASN:HD21	1:B:778:LYS:HZ1	1.44	0.65
1:A:679:GLN:NE2	1:A:683:ARG:HH22	1.94	0.65
1:A:1279:ARG:HH21	1:A:1290:LYS:HD3	1.61	0.65
1:A:666:ILE:CD1	1:A:807:VAL:HG13	2.27	0.64
1:B:426:ARG:HD3	1:B:1212:HIS:CG	2.32	0.64
1:B:123:MET:HE2	1:B:159:PHE:CD2	2.33	0.64
1:B:1208:MET:HE2	1:B:1234:SER:HB3	1.79	0.64
1:B:271:ASN:HB3	1:B:683:ARG:HH11	1.62	0.64
1:B:646:THR:HG22	1:B:647:GLY:N	2.07	0.64
1:A:646:THR:HG22	1:A:647:GLY:N	2.09	0.63
1:B:531:LEU:CA	1:B:540:PRO:HD2	2.28	0.62
1:A:646:THR:HG23	8:A:7667:HOH:O	1.99	0.62
1:B:1082:SER:HB2	3:B:6003:PO4:O2	1.98	0.62
1:B:271:ASN:CG	1:B:683:ARG:HD3	2.19	0.62
1:B:601:ASN:H	1:B:601:ASN:HD22	1.48	0.62
1:A:93:ASN:OD1	1:A:95:GLN:HG3	1.99	0.61
1:B:715:GLU:OE2	1:B:895:ARG:HD2	2.01	0.61
1:A:882:LEU:O	1:A:954:HIS:HE1	1.83	0.61
1:A:856:VAL:HG12	1:A:945:ASN:OD1	2.01	0.60
6:B:3003:FAD:O2B	6:B:3003:FAD:C3B	2.45	0.60
1:B:544:SER:HB2	1:B:994:LYS:HG3	1.84	0.60
1:A:240:THR:OG1	1:A:243:GLU:HG3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:603:LEU:HD21	1:B:821:ARG:NH2	2.18	0.59
1:B:650:ASN:ND2	1:B:778:LYS:NZ	2.49	0.59
1:B:271:ASN:HB3	1:B:683:ARG:NH1	2.17	0.59
1:A:1004:LYS:HG3	1:A:1155:TYR:CE2	2.38	0.59
1:B:761:GLU:HA	1:B:788:VAL:HG13	1.85	0.59
1:A:616:LYS:HD3	1:A:659:GLU:HB3	1.85	0.58
1:B:812:LEU:HD21	1:B:823:VAL:O	2.03	0.58
1:A:1311:GLN:HB2	1:A:1317:VAL:HG13	1.85	0.58
1:A:601:ASN:H	1:A:601:ASN:HD22	1.51	0.58
1:A:271:ASN:OD1	1:A:683:ARG:CZ	2.51	0.58
1:A:164:LYS:NZ	1:A:164:LYS:HB2	2.19	0.57
1:B:478:ASN:HD21	1:B:480:GLU:HG3	1.68	0.57
1:B:130:GLN:HE21	1:B:132:GLU:N	1.96	0.57
1:B:1088:GLN:HG2	1:B:1133:TYR:CE1	2.39	0.57
1:B:123:MET:CE	1:B:138:ILE:HG23	2.33	0.57
1:B:486:CYS:HA	1:B:512:LEU:HD22	1.85	0.57
1:A:370:LYS:HE2	1:A:383:ARG:HE	1.69	0.57
1:B:606:ARG:HD3	1:B:679:GLN:HA	1.86	0.57
1:B:646:THR:HG23	8:B:7280:HOH:O	2.05	0.57
1:B:886:ASP:OD1	1:B:1004:LYS:NZ	2.38	0.57
1:A:306:LEU:HD23	1:A:306:LEU:O	2.05	0.56
1:B:749:THR:O	1:B:812:LEU:HD22	2.05	0.56
1:A:880:ARG:HD2	1:A:914:PHE:HB3	1.85	0.56
1:B:446:ILE:O	1:B:446:ILE:HG12	2.04	0.56
1:B:954:HIS:CD2	1:B:954:HIS:H	2.23	0.56
1:A:216:LEU:O	1:A:219:LYS:HB3	2.06	0.56
1:B:1203:LEU:CD2	1:B:1208:MET:HE3	2.35	0.56
1:B:132:GLU:HB3	1:B:164:LYS:CG	2.36	0.56
1:B:446:ILE:HG12	1:B:477:TRP:H	1.69	0.56
1:B:4:ASP:HB3	8:B:7379:HOH:O	2.04	0.56
1:B:880:ARG:HD2	1:B:914:PHE:HB3	1.87	0.56
1:A:1311:GLN:HG3	1:A:1317:VAL:CG1	2.36	0.55
1:B:882:LEU:O	1:B:954:HIS:HE1	1.89	0.55
1:B:321:GLN:HG2	1:B:413:GLU:CD	2.27	0.55
1:B:246:ASP:OD2	1:B:376:ARG:HD2	2.06	0.55
1:A:135:VAL:HG23	1:A:165:ASP:HB3	1.88	0.55
1:B:577:LEU:HD12	1:B:578:PRO:HD2	1.88	0.55
1:A:531:LEU:HD12	1:A:534:MET:SD	2.47	0.55
1:B:1250:LYS:CE	1:B:1251:ARG:HG3	2.35	0.55
1:B:666:ILE:CD1	1:B:807:VAL:HG13	2.37	0.55
1:A:59:ASP:HB3	1:A:62:GLN:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1208:MET:CE	1:B:1234:SER:HB3	2.37	0.55
1:B:640:VAL:HG23	1:B:640:VAL:O	2.07	0.55
1:B:55:ILE:HG23	1:B:83:VAL:CG1	2.36	0.55
1:B:900:ILE:HD12	1:B:900:ILE:N	2.21	0.55
1:A:58:TYR:OH	1:A:63:ASN:HA	2.07	0.54
1:B:135:VAL:HG23	1:B:165:ASP:HA	1.89	0.54
1:B:123:MET:HE3	1:B:138:ILE:HG23	1.88	0.54
1:B:132:GLU:O	1:B:164:LYS:HE3	2.08	0.54
1:B:998:LEU:HD13	1:B:1161:GLU:HB2	1.89	0.54
1:A:58:TYR:CE2	1:A:219:LYS:HG3	2.43	0.54
1:B:370:LYS:HD2	1:B:407:GLU:OE1	2.08	0.54
1:B:164:LYS:HB2	1:B:164:LYS:NZ	2.22	0.54
1:B:332:GLN:CA	1:B:332:GLN:HE21	2.18	0.54
1:B:887:ASN:O	1:B:1004:LYS:HE2	2.08	0.54
1:B:55:ILE:HG23	1:B:83:VAL:HG13	1.90	0.54
1:A:785:ASN:C	1:A:785:ASN:HD22	2.12	0.53
1:B:82:HIS:CE1	1:B:218:LEU:HD13	2.43	0.53
1:A:812:LEU:HD11	1:A:823:VAL:C	2.27	0.53
1:B:296:ILE:CD1	1:B:314:GLU:HG3	2.39	0.53
1:B:332:GLN:NE2	1:B:332:GLN:HA	2.21	0.53
1:A:666:ILE:HD12	1:A:807:VAL:HG13	1.89	0.53
1:A:469:THR:N	1:A:470:PRO:HD2	2.23	0.53
1:A:508:ARG:CZ	1:A:1315:LEU:HD11	2.39	0.53
1:A:972:ILE:HG13	1:A:973:ALA:N	2.24	0.53
1:A:911:PHE:O	1:A:912:ARG:C	2.46	0.53
1:B:1317:VAL:HG23	1:B:1318:THR:N	2.24	0.52
1:A:874:SER:HB3	1:A:900:ILE:HG21	1.90	0.52
1:A:785:ASN:HD22	1:A:786:ARG:N	2.07	0.52
1:B:923:ALA:HA	1:B:926:TRP:NE1	2.25	0.52
1:A:1082:SER:HB2	3:A:6002:PO4:O4	2.09	0.52
1:A:749:THR:O	1:A:812:LEU:HD22	2.08	0.52
1:B:388:PHE:HA	1:B:396:LEU:HG	1.92	0.52
1:B:911:PHE:O	1:B:912:ARG:C	2.47	0.52
1:B:812:LEU:HD11	1:B:823:VAL:C	2.29	0.52
1:B:1091:TYR:O	1:B:1095:GLN:HG2	2.09	0.52
1:B:1053:ALA:O	1:B:1098:LEU:HD11	2.10	0.52
1:A:900:ILE:HD12	1:A:900:ILE:N	2.25	0.52
1:B:478:ASN:C	1:B:478:ASN:HD22	2.12	0.52
1:A:124:TYR:OH	1:A:208:GLU:HG3	2.09	0.52
1:B:240:THR:OG1	1:B:243:GLU:HG3	2.10	0.51
1:A:555:ALA:O	1:A:1238:GLU:HA	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:667:ILE:HD13	1:A:687:ILE:HD13	1.92	0.51
1:A:111:GLN:NE2	1:A:150:THR:HA	2.25	0.51
1:A:581:ALA:O	1:A:585:GLN:HG3	2.09	0.51
1:B:157:GLN:HA	1:B:160:ARG:NH1	2.26	0.51
1:B:62:GLN:OE1	1:B:64:LYS:HE3	2.10	0.51
1:B:123:MET:HE3	1:B:159:PHE:HB3	1.93	0.51
1:A:812:LEU:HD11	1:A:823:VAL:HG12	1.93	0.51
1:A:1221:THR:CG2	1:A:1227:TYR:HB2	2.41	0.51
1:A:1053:ALA:O	1:A:1098:LEU:HD11	2.11	0.51
1:B:666:ILE:HD11	1:B:807:VAL:HG13	1.91	0.51
1:B:601:ASN:N	1:B:601:ASN:HD22	2.07	0.51
1:A:267:MET:HE1	8:A:7168:HOH:O	2.10	0.51
1:A:487:ALA:CA	1:A:1318:THR:HG23	2.41	0.51
1:A:812:LEU:CD1	1:A:823:VAL:HG12	2.40	0.50
1:A:601:ASN:N	1:A:601:ASN:HD22	2.09	0.50
1:A:1054:LEU:O	1:A:1055:LYS:HB2	2.11	0.50
1:B:469:THR:N	1:B:470:PRO:HD2	2.26	0.50
1:B:764:VAL:O	1:B:791:VAL:HG22	2.10	0.50
1:A:695:ILE:HG23	1:A:700:ASP:HB3	1.92	0.50
1:B:132:GLU:HB3	1:B:164:LYS:HG3	1.92	0.50
1:B:123:MET:HE2	1:B:142:PHE:HZ	1.75	0.50
1:A:32:ARG:NH1	1:A:675:PRO:HD2	2.27	0.50
1:B:969:ASP:O	1:B:972:ILE:HG12	2.12	0.50
1:A:253:ASP:N	1:A:253:ASP:OD2	2.45	0.50
1:A:321:GLN:HG2	1:A:413:GLU:OE1	2.12	0.50
1:B:670:VAL:HG11	1:B:681:ALA:HB3	1.92	0.50
1:A:995:LYS:NZ	1:A:1284:GLN:NE2	2.60	0.50
1:A:426:ARG:HD3	1:A:1212:HIS:CG	2.46	0.50
1:A:3:ALA:CB	1:A:227:ARG:H	2.11	0.50
1:A:478:ASN:ND2	1:A:480:GLU:H	2.10	0.50
1:B:426:ARG:HG2	1:B:426:ARG:O	2.11	0.49
1:A:1287:ASP:O	1:A:1288:ASN:HB2	2.11	0.49
1:A:670:VAL:HG11	1:A:681:ALA:HB3	1.93	0.49
1:A:1134:LYS:HD3	1:B:1124:ALA:HB3	1.92	0.49
1:B:761:GLU:HG3	1:B:788:VAL:HG13	1.93	0.49
1:B:1086:ASN:O	1:B:1090:VAL:HG23	2.11	0.49
1:A:1037:GLU:HB2	1:A:1043:HIS:CD2	2.47	0.49
1:B:785:ASN:HD22	1:B:786:ARG:N	2.10	0.49
1:A:1004:LYS:HG3	1:A:1155:TYR:HE2	1.77	0.49
1:A:537:LYS:O	1:A:538:LEU:CB	2.60	0.49
1:A:387:THR:O	1:A:396:LEU:HD21	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1311:GLN:HG3	1:A:1317:VAL:HG13	1.93	0.49
1:B:733:GLU:OE1	1:B:845:LYS:HE2	2.12	0.49
1:A:1003:THR:HG22	1:A:1266:LEU:HD21	1.94	0.49
1:B:909:THR:OG1	1:B:910:ALA:N	2.43	0.49
1:B:655:PHE:HE2	1:B:814:LEU:HD23	1.77	0.49
1:B:749:THR:HG22	1:B:812:LEU:HD22	1.93	0.49
1:B:812:LEU:HD11	1:B:824:ARG:N	2.27	0.49
1:B:733:GLU:HG2	1:B:845:LYS:HG2	1.95	0.49
1:A:311:LEU:O	1:A:315:ILE:HG13	2.13	0.49
1:A:1107:LYS:O	1:A:1108:LYS:HD2	2.13	0.49
1:B:266:GLU:O	1:B:270:LYS:HB2	2.13	0.48
1:A:756:GLU:OE2	1:B:793:ARG:NH2	2.46	0.48
1:B:605:LEU:C	1:B:605:LEU:HD23	2.33	0.48
1:B:785:ASN:HD22	1:B:785:ASN:C	2.15	0.48
1:A:954:HIS:H	1:A:954:HIS:CD2	2.30	0.48
1:B:422:GLN:HG2	1:B:424:SER:H	1.78	0.48
1:B:402:ILE:HD12	1:B:402:ILE:C	2.34	0.48
1:A:558:GLN:HB3	1:A:1192:ILE:HD13	1.95	0.48
1:B:601:ASN:H	1:B:601:ASN:ND2	2.11	0.48
1:B:880:ARG:HD2	1:B:914:PHE:O	2.14	0.48
1:B:1107:LYS:C	1:B:1109:PRO:HD3	2.33	0.48
1:A:431:ALA:HB2	1:A:501:GLY:HA3	1.93	0.48
1:A:1107:LYS:C	1:A:1108:LYS:HD2	2.34	0.48
1:A:785:ASN:ND2	1:A:786:ARG:HG2	2.29	0.48
1:A:1132:PHE:CG	1:B:1126:SER:HB2	2.48	0.48
1:B:1313:THR:O	1:B:1317:VAL:HG22	2.14	0.48
1:A:62:GLN:O	1:A:64:LYS:HG3	2.13	0.48
1:A:711:GLU:HA	1:A:899:ARG:CD	2.44	0.48
1:B:1214:SER:HB3	1:B:1220:HIS:NE2	2.29	0.48
1:B:164:LYS:O	1:B:165:ASP:HB2	2.14	0.48
1:A:306:LEU:HD23	1:A:306:LEU:C	2.34	0.48
1:B:531:LEU:CB	1:B:540:PRO:HD2	2.43	0.47
1:A:667:ILE:CD1	1:A:687:ILE:HD13	2.43	0.47
1:B:245:LEU:HD22	1:B:375:SER:HA	1.95	0.47
1:B:1045:LYS:HE3	1:B:1190:ILE:HG21	1.97	0.47
1:B:646:THR:HG21	8:B:7201:HOH:O	2.14	0.47
1:A:552:ASP:HB2	1:A:1237:ILE:HD13	1.95	0.47
1:A:711:GLU:HA	1:A:899:ARG:HD3	1.97	0.47
1:B:528:ARG:HG2	1:B:528:ARG:HH11	1.80	0.47
1:B:874:SER:HB3	1:B:900:ILE:HG21	1.96	0.47
1:A:909:THR:OG1	1:A:910:ALA:N	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:ARG:C	1:B:153:ARG:HD2	2.35	0.47
1:B:1007:ILE:O	1:B:1008:SER:CB	2.63	0.47
1:A:557:VAL:HG12	1:A:1240:ARG:CG	2.41	0.47
1:A:236:ILE:HD12	1:A:247:LEU:HD11	1.97	0.46
1:B:657:LYS:O	1:B:658:ASP:HB2	2.14	0.46
1:B:1203:LEU:HD21	1:B:1208:MET:HE3	1.96	0.46
1:A:372:THR:HG21	1:A:404:LEU:HD23	1.96	0.46
1:A:370:LYS:CE	1:A:383:ARG:HH21	2.29	0.46
1:A:217:ARG:C	1:A:219:LYS:H	2.18	0.46
1:B:441:PHE:CZ	1:B:526:LEU:HD11	2.50	0.46
1:A:163:ALA:C	1:A:165:ASP:H	2.19	0.46
1:A:923:ALA:HA	1:A:926:TRP:NE1	2.30	0.46
1:A:5:GLU:HG2	8:A:7612:HOH:O	2.16	0.46
1:B:641:PRO:HG2	1:B:780:LEU:HA	1.96	0.46
1:A:487:ALA:CB	1:A:1318:THR:HG23	2.45	0.46
1:A:400:GLU:H	1:A:400:GLU:CD	2.20	0.46
1:B:637:ALA:O	1:B:640:VAL:HG22	2.16	0.46
1:B:467:LYS:HB2	1:B:492:GLU:CD	2.36	0.46
1:A:1007:ILE:O	1:A:1008:SER:CB	2.64	0.46
1:A:964:LEU:HB3	1:A:965:PRO:HD3	1.97	0.46
1:B:1209:GLU:O	1:B:1298:PRO:HG3	2.16	0.45
1:A:812:LEU:HD21	1:A:823:VAL:O	2.16	0.45
1:B:545:ALA:HB2	1:B:993:TRP:HB2	1.97	0.45
1:B:231:GLU:OE2	1:B:680:ARG:NH1	2.49	0.45
1:B:646:THR:CG2	1:B:647:GLY:H	2.09	0.45
1:A:646:THR:HG21	8:A:7078:HOH:O	2.15	0.45
1:B:1318:THR:HG22	1:B:1320:VAL:H	1.80	0.45
1:A:1221:THR:HG22	1:A:1227:TYR:HB2	1.97	0.45
1:B:1281:ALA:O	1:B:1284:GLN:HB3	2.16	0.45
1:B:1250:LYS:HE3	1:B:1251:ARG:HG3	1.97	0.45
1:B:296:ILE:HD11	1:B:314:GLU:HG3	1.98	0.45
1:B:875:ARG:O	1:B:879:GLU:HG3	2.16	0.45
1:B:812:LEU:HD11	1:B:823:VAL:HG12	1.98	0.45
1:B:711:GLU:HA	1:B:899:ARG:HD2	1.97	0.45
1:B:1252:ALA:HB3	1:B:1256:SER:O	2.17	0.45
1:B:481:LEU:HD23	1:B:481:LEU:C	2.37	0.45
1:B:1203:LEU:HD23	1:B:1203:LEU:C	2.37	0.45
1:A:255:LYS:HG3	1:A:274:PHE:CD1	2.52	0.45
1:A:373:LEU:HD22	1:A:397:LEU:HD11	1.98	0.45
1:A:256:LEU:HD22	1:A:278:VAL:CG1	2.47	0.45
1:B:606:ARG:CD	1:B:679:GLN:HA	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:ALA:HB3	1:A:531:LEU:HD23	1.99	0.45
1:B:964:LEU:HB3	1:B:965:PRO:HD3	1.97	0.45
1:B:751:ALA:H	1:B:812:LEU:HD21	1.82	0.45
1:A:751:ALA:H	1:A:812:LEU:HD21	1.82	0.44
1:A:64:LYS:NZ	1:A:64:LYS:HB3	2.32	0.44
1:B:241:MET:HE1	1:B:283:ILE:HG21	1.99	0.44
1:B:263:ILE:HD11	6:B:3003:FAD:H3B	1.99	0.44
1:A:130:GLN:O	1:A:133:PRO:HD3	2.17	0.44
1:B:650:ASN:ND2	1:B:778:LYS:HZ3	2.15	0.44
1:B:557:VAL:HG22	1:B:1240:ARG:HG2	1.99	0.44
1:A:504:VAL:HG23	1:A:505:GLU:N	2.33	0.44
1:B:711:GLU:HA	1:B:899:ARG:CD	2.47	0.44
1:B:986:LYS:O	1:B:990:GLU:HG3	2.17	0.44
1:B:130:GLN:NE2	1:B:132:GLU:H	1.99	0.44
1:B:400:GLU:HB2	8:B:7626:HOH:O	2.18	0.44
1:A:1088:GLN:NE2	8:A:7582:HOH:O	2.49	0.44
1:B:939:GLU:CG	1:B:977:TYR:CE2	2.97	0.44
1:A:1314:THR:O	1:A:1315:LEU:HB2	2.17	0.44
1:A:58:TYR:CZ	1:A:63:ASN:HA	2.52	0.44
1:A:1086:ASN:O	1:A:1090:VAL:HG23	2.18	0.44
1:A:952:LEU:HD23	1:A:958:LYS:HA	2.00	0.44
1:A:1088:GLN:HG2	1:A:1133:TYR:CE1	2.50	0.44
1:A:1034:GLY:HA3	8:A:7049:HOH:O	2.17	0.44
1:B:753:PRO:HD3	1:B:816:ALA:HB1	1.99	0.44
1:A:939:GLU:HG2	1:A:977:TYR:CZ	2.52	0.44
1:B:812:LEU:CD1	1:B:823:VAL:HG12	2.48	0.44
1:A:880:ARG:HD2	1:A:914:PHE:O	2.18	0.44
1:A:1180:MET:HE1	1:A:1263:PRO:HA	1.99	0.44
1:A:962:PHE:CE2	1:A:965:PRO:HD3	2.52	0.44
1:A:605:LEU:C	1:A:605:LEU:HD23	2.38	0.44
1:A:95:GLN:OE1	1:A:96:LYS:HB2	2.17	0.43
1:A:211:PHE:CD2	1:A:216:LEU:HD13	2.53	0.43
1:A:756:GLU:CD	1:B:793:ARG:HH22	2.21	0.43
1:B:793:ARG:HG2	8:B:7042:HOH:O	2.18	0.43
1:A:767:GLN:HG3	1:A:801:LYS:HB2	1.99	0.43
1:A:641:PRO:HG2	1:A:780:LEU:HA	1.99	0.43
1:B:128:ARG:HB3	1:B:128:ARG:NH1	2.33	0.43
1:A:324:GLU:HB2	1:A:411:SER:CB	2.48	0.43
1:A:503:MET:HG2	1:A:1302:GLU:OE2	2.18	0.43
1:A:751:ALA:N	1:A:812:LEU:HD21	2.33	0.43
1:A:315:ILE:HD13	1:A:327:ARG:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1034:GLY:HA3	8:B:7040:HOH:O	2.19	0.43
1:A:601:ASN:ND2	1:A:601:ASN:H	2.16	0.43
1:A:601:ASN:O	1:A:821:ARG:HD2	2.19	0.43
1:B:1088:GLN:CG	1:B:1133:TYR:CD1	2.94	0.43
1:B:751:ALA:N	1:B:812:LEU:HD21	2.34	0.43
1:B:151:GLY:HA2	1:B:1200:VAL:HG21	1.99	0.43
1:B:153:ARG:N	1:B:154:PRO:HD2	2.34	0.43
1:B:504:VAL:HG23	1:B:505:GLU:N	2.34	0.43
1:B:357:ILE:CD1	1:B:429:ASP:HA	2.49	0.43
1:A:388:PHE:HA	1:A:396:LEU:CG	2.44	0.43
1:A:217:ARG:C	1:A:219:LYS:N	2.72	0.43
1:B:29:TYR:CE1	1:B:33:LYS:HG2	2.54	0.43
1:A:753:PRO:HD3	1:A:816:ALA:HB1	1.99	0.43
1:B:1300:THR:O	1:B:1304:ILE:HG13	2.18	0.43
1:A:3:ALA:HA	1:A:226:LEU:HD22	2.00	0.43
1:A:263:ILE:HG22	1:A:267:MET:CE	2.48	0.43
1:A:616:LYS:HG2	1:A:692:LEU:HD11	2.02	0.42
1:A:251:HIS:C	1:A:253:ASP:H	2.23	0.42
1:A:1203:LEU:HD23	1:A:1203:LEU:C	2.40	0.42
1:B:785:ASN:ND2	1:B:786:ARG:HG2	2.34	0.42
1:B:252:PRO:CG	1:B:400:GLU:HG2	2.39	0.42
1:B:1151:HIS:NE2	1:B:1251:ARG:HB3	2.33	0.42
1:A:688:THR:HG23	8:A:7329:HOH:O	2.19	0.42
1:A:481:LEU:HD23	1:A:481:LEU:C	2.38	0.42
1:A:1088:GLN:HG2	1:A:1133:TYR:CG	2.51	0.42
1:B:82:HIS:NE2	1:B:218:LEU:HD13	2.33	0.42
1:B:256:LEU:HD22	1:B:278:VAL:HG13	2.00	0.42
1:A:644:ASN:O	1:A:653:THR:HA	2.20	0.42
1:A:666:ILE:HD11	1:A:807:VAL:CG1	2.49	0.42
1:A:926:TRP:O	1:A:930:VAL:HG23	2.19	0.42
1:B:1300:THR:HB	1:B:1301:PRO:HD2	2.02	0.42
1:B:164:LYS:HB2	1:B:164:LYS:HZ2	1.85	0.42
1:A:1143:GLU:OE1	1:A:1143:GLU:N	2.48	0.42
1:A:698:ILE:O	1:A:702:ILE:HG13	2.20	0.42
1:A:1250:LYS:CE	1:A:1251:ARG:HG3	2.49	0.42
1:A:749:THR:HG23	1:A:764:VAL:HG22	2.02	0.42
1:B:640:VAL:CG2	1:B:640:VAL:O	2.68	0.42
1:B:783:PRO:HB2	1:B:785:ASN:ND2	2.35	0.42
1:A:29:TYR:CZ	1:A:33:LYS:HG2	2.55	0.42
1:A:657:LYS:O	1:A:658:ASP:HB2	2.20	0.42
1:A:532:GLU:OE1	1:A:537:LYS:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:ARG:NE	1:A:208:GLU:HG2	2.35	0.41
1:B:508:ARG:HG2	1:B:508:ARG:HH11	1.84	0.41
1:A:336:LEU:HG	6:A:2003:FAD:C4	2.49	0.41
1:B:94:THR:HG21	1:B:584:MET:HG2	2.02	0.41
1:A:251:HIS:C	1:A:253:ASP:N	2.72	0.41
1:B:785:ASN:ND2	1:B:786:ARG:NH1	2.49	0.41
1:A:711:GLU:CA	1:A:899:ARG:HD3	2.50	0.41
1:A:1180:MET:HE1	1:A:1266:LEU:HD12	2.01	0.41
1:B:1199:PHE:CE1	1:B:1267:ALA:HA	2.55	0.41
1:B:531:LEU:C	1:B:531:LEU:HD23	2.41	0.41
1:B:123:MET:HE1	1:B:138:ILE:HG23	2.00	0.41
1:B:1004:LYS:HB3	1:B:1004:LYS:HE2	1.86	0.41
1:A:297:SER:HA	1:A:407:GLU:HA	2.03	0.41
1:A:153:ARG:N	1:A:154:PRO:HD2	2.35	0.41
1:A:1279:ARG:NH2	1:A:1290:LYS:HD3	2.33	0.41
1:A:1198:ALA:HB3	1:A:1263:PRO:HB2	2.02	0.41
1:B:262:GLU:O	1:B:266:GLU:HG3	2.20	0.41
1:B:1291:GLN:HG2	1:B:1292:LEU:N	2.36	0.41
1:A:655:PHE:HE2	1:A:814:LEU:HD23	1.85	0.41
1:A:891:ILE:HA	1:A:892:PRO:HD3	1.91	0.41
1:A:719:LEU:HD11	1:A:895:ARG:CB	2.46	0.41
1:A:708:TYR:CE1	1:A:902:LYS:HA	2.56	0.41
1:A:539:ASP:HB3	1:A:542:PHE:CD1	2.56	0.41
1:A:233:VAL:HG12	1:A:234:THR:N	2.35	0.41
1:B:130:GLN:O	1:B:133:PRO:HD3	2.21	0.41
1:B:1102:GLU:HB3	1:B:1103:PRO:CD	2.48	0.41
1:B:1200:VAL:O	1:B:1203:LEU:HB3	2.21	0.41
1:A:46:GLY:CA	5:A:2002:FES:S1	3.09	0.41
1:B:116:THR:HB	1:B:117:PRO:HD3	2.03	0.41
1:A:1105:LYS:HB2	1:A:1105:LYS:HE3	1.91	0.41
1:B:1105:LYS:HA	1:B:1116:TRP:NE1	2.36	0.41
1:A:1214:SER:HB3	1:A:1220:HIS:NE2	2.36	0.41
1:B:311:LEU:O	1:B:315:ILE:HG13	2.21	0.41
1:A:116:THR:HB	1:A:117:PRO:HD3	2.03	0.41
1:B:418:SER:HB2	1:B:518:PHE:CD1	2.56	0.41
1:A:610:SER:HB2	1:A:660:VAL:HG11	2.02	0.41
1:A:3:ALA:HA	1:A:226:LEU:CD2	2.51	0.41
1:A:764:VAL:O	1:A:791:VAL:HG22	2.21	0.41
1:B:531:LEU:HB2	1:B:540:PRO:HD2	2.03	0.41
1:B:504:VAL:HG22	8:B:7235:HOH:O	2.21	0.41
1:B:868:GLY:HA3	1:B:907:SER:HA	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1069:ASN:HD22	1:A:1069:ASN:C	2.24	0.41
1:A:1252:ALA:HB3	1:A:1256:SER:O	2.20	0.41
1:A:132:GLU:O	1:A:164:LYS:HE3	2.21	0.40
1:B:531:LEU:HG	1:B:540:PRO:HB2	2.03	0.40
1:B:294:GLU:HG3	1:B:370:LYS:NZ	2.36	0.40
1:A:1151:HIS:NE2	1:A:1251:ARG:HB3	2.36	0.40
1:A:221:THR:HA	1:A:222:PRO:HD3	1.93	0.40
1:A:783:PRO:HB3	1:B:1028:SER:HB3	2.03	0.40
1:A:1311:GLN:CG	1:A:1317:VAL:HG13	2.52	0.40
1:B:132:GLU:HB3	1:B:164:LYS:HD3	2.02	0.40
1:A:1091:TYR:O	1:A:1095:GLN:HG2	2.22	0.40
1:A:473:LEU:O	1:A:474:SER:CB	2.69	0.40
1:A:134:THR:OG1	1:A:137:GLU:HG3	2.22	0.40
1:A:132:GLU:HB3	1:A:164:LYS:HD3	2.04	0.40
1:B:478:ASN:C	1:B:478:ASN:ND2	2.75	0.40
1:A:539:ASP:HA	1:A:540:PRO:HD3	1.97	0.40
1:B:46:GLY:HA2	5:B:2002:FES:S1	2.62	0.40
1:A:334:ARG:HB3	1:A:334:ARG:NH1	2.36	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	1287/1331 (97%)	1220 (95%)	57 (4%)	10 (1%)	24	26
1	B	1273/1331 (96%)	1220 (96%)	46 (4%)	7 (0%)	34	39
All	All	2560/2662 (96%)	2440 (95%)	103 (4%)	17 (1%)	26	30

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	1008	SER
1	A	1287	ASP
1	A	1288	ASN
1	B	4	ASP
1	B	1008	SER
1	A	62	GLN
1	A	912	ARG
1	B	912	ARG
1	B	1286	GLY
1	A	797	GLY
1	B	376	ARG
1	B	797	GLY
1	A	538	LEU
1	A	474	SER
1	B	1139	GLY
1	A	1012	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	1089/1123 (97%)	1064 (98%)	25 (2%)	58 73
1	B	1079/1123 (96%)	1058 (98%)	21 (2%)	65 79
All	All	2168/2246 (96%)	2122 (98%)	46 (2%)	61 76

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	GLN
1	A	208	GLU
1	A	247	LEU
1	A	253	ASP
1	A	255	LYS
1	A	256	LEU
1	A	400	GLU

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Mol	Chain	Res	Type
1	A	432	LYS
1	A	480	GLU
1	A	551	LYS
1	A	572	MET
1	A	601	ASN
1	A	650	ASN
1	A	743	TYR
1	A	785	ASN
1	A	911	PHE
1	A	939	GLU
1	A	1002	PRO
1	A	1031	LEU
1	A	1069	ASN
1	A	1085	LEU
1	A	1177	ASP
1	A	1239	PHE
1	A	1250	LYS
1	A	1276	ASP
1	B	199	ASP
1	B	253	ASP
1	B	255	LYS
1	B	306	LEU
1	B	332	GLN
1	B	350	ASN
1	B	383	ARG
1	B	478	ASN
1	B	480	GLU
1	B	572	MET
1	B	601	ASN
1	B	743	TYR
1	B	785	ASN
1	B	869	ASN
1	B	911	PHE
1	B	1069	ASN
1	B	1072	PRO
1	B	1085	LEU
1	B	1239	PHE
1	B	1250	LYS
1	B	1276	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	71	ASN
1	A	111	GLN
1	A	130	GLN
1	A	145	ASN
1	A	350	ASN
1	A	472	GLN
1	A	478	ASN
1	A	583	ASN
1	A	585	GLN
1	A	601	ASN
1	A	642	ASN
1	A	650	ASN
1	A	679	GLN
1	A	747	ASN
1	A	785	ASN
1	A	954	HIS
1	A	1069	ASN
1	A	1088	GLN
1	A	1284	GLN
1	B	63	ASN
1	B	71	ASN
1	B	130	GLN
1	B	145	ASN
1	B	223	GLN
1	B	332	GLN
1	B	350	ASN
1	B	386	HIS
1	B	478	ASN
1	B	583	ASN
1	B	585	GLN
1	B	601	ASN
1	B	642	ASN
1	B	650	ASN
1	B	747	ASN
1	B	785	ASN
1	B	869	ASN
1	B	954	HIS
1	B	1069	ASN
1	B	1086	ASN
1	B	1284	GLN

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 25 ligands modelled in this entry, 4 are monoatomic - leaving 21 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	$\#\|Z\|>2$
5	FES	A	2001	1	0,4,4	0.00	-	0,4,4	0.00	-
5	FES	A	2002	1	0,4,4	0.00	-	0,4,4	0.00	-
6	FAD	A	2003	-	48,58,58	3.46	14 (29%)	54,89,89	2.64	15 (27%)
7	URC	A	4001	-	12,13,13	4.82	4 (33%)	10,19,19	4.30	4 (40%)
2	BCT	A	5001	-	0,3,3	0.00	-	0,3,3	0.00	-
3	PO4	A	6001	-	4,4,4	1.12	0	6,6,6	0.27	0
3	PO4	A	6002	-	4,4,4	1.18	0	6,6,6	0.27	0
3	PO4	A	6004	-	4,4,4	1.08	0	6,6,6	0.27	0
3	PO4	A	6006	-	4,4,4	1.12	0	6,6,6	0.27	0
3	PO4	A	6008	-	4,4,4	1.09	0	6,6,6	0.27	0
3	PO4	A	6009	-	4,4,4	1.08	0	6,6,6	0.27	0
5	FES	B	2001	1	0,4,4	0.00	-	0,4,4	0.00	-
5	FES	B	2002	1	0,4,4	0.00	-	0,4,4	0.00	-
6	FAD	B	3003	-	48,58,58	4.35	22 (45%)	54,89,89	2.62	12 (22%)
7	URC	B	4002	-	12,13,13	4.78	5 (41%)	10,19,19	4.32	4 (40%)
2	BCT	B	5002	-	0,3,3	0.00	-	0,3,3	0.00	-
3	PO4	B	6003	-	4,4,4	1.22	0	6,6,6	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	PO4	B	6005	-	4,4,4	1.12	0	6,6,6	0.27	0
3	PO4	B	6007	-	4,4,4	1.14	0	6,6,6	0.27	0
3	PO4	B	6010	-	4,4,4	1.12	0	6,6,6	0.27	0
3	PO4	B	6011	-	4,4,4	1.12	0	6,6,6	0.27	0

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
5	FES	A	2001	1	-	0/0/4/4	0/1/1/1
5	FES	A	2002	1	-	0/0/4/4	0/1/1/1
6	FAD	A	2003	-	-	0/30/50/50	0/6/6/6
7	URC	A	4001	-	-	0/0/24/24	0/2/2/2
2	BCT	A	5001	-	-	0/0/0/0	0/0/0/0
3	PO4	A	6001	-	-	0/0/0/0	0/0/0/0
3	PO4	A	6002	-	-	0/0/0/0	0/0/0/0
3	PO4	A	6004	-	-	0/0/0/0	0/0/0/0
3	PO4	A	6006	-	-	0/0/0/0	0/0/0/0
3	PO4	A	6008	-	-	0/0/0/0	0/0/0/0
3	PO4	A	6009	-	-	0/0/0/0	0/0/0/0
5	FES	B	2001	1	-	0/0/4/4	0/1/1/1
5	FES	B	2002	1	-	0/0/4/4	0/1/1/1
6	FAD	B	3003	-	-	0/30/50/50	0/6/6/6
7	URC	B	4002	-	-	0/0/24/24	0/2/2/2
2	BCT	B	5002	-	-	0/0/0/0	0/0/0/0
3	PO4	B	6003	-	-	0/0/0/0	0/0/0/0
3	PO4	B	6005	-	-	0/0/0/0	0/0/0/0
3	PO4	B	6007	-	-	0/0/0/0	0/0/0/0
3	PO4	B	6010	-	-	0/0/0/0	0/0/0/0
3	PO4	B	6011	-	-	0/0/0/0	0/0/0/0

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	3003	FAD	C5'-C4'	-20.09	1.20	1.51
6	A	2003	FAD	C5'-C4'	-14.56	1.29	1.51
7	A	4001	URC	C4-N9	-11.80	1.30	1.44
7	B	4002	URC	C4-N9	-11.69	1.30	1.44
6	A	2003	FAD	O2B-C2B	-9.06	1.21	1.43
7	A	4001	URC	C4-N3	-8.96	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	4002	URC	C4-N3	-8.81	1.35	1.46
6	B	3003	FAD	O2B-C2B	-7.47	1.25	1.43
7	A	4001	URC	C5-N7	-7.01	1.30	1.45
7	B	4002	URC	C5-N7	-6.89	1.30	1.45
6	B	3003	FAD	C5B-C4B	-5.42	1.34	1.51
6	A	2003	FAD	O5'-C5'	-3.76	1.29	1.44
6	B	3003	FAD	P-O5'	-2.74	1.46	1.59
6	B	3003	FAD	PA-O2A	-2.49	1.44	1.54
6	A	2003	FAD	PA-O2A	-2.47	1.44	1.54
6	B	3003	FAD	O3B-C3B	-2.38	1.37	1.43
6	B	3003	FAD	O5'-C5'	-2.31	1.35	1.44
7	B	4002	URC	C8-N7	-2.24	1.32	1.35
7	B	4002	URC	C8-N9	-2.23	1.32	1.35
7	A	4001	URC	C8-N9	-2.17	1.32	1.35
6	A	2003	FAD	O3B-C3B	-2.11	1.37	1.43
6	B	3003	FAD	PA-O5B	-2.06	1.49	1.59
6	A	2003	FAD	C4A-N3A	2.01	1.38	1.35
6	B	3003	FAD	C2A-N3A	2.11	1.35	1.32
6	B	3003	FAD	O5B-C5B	2.27	1.54	1.44
6	A	2003	FAD	C6-C7	2.28	1.44	1.37
6	B	3003	FAD	C4A-N3A	2.43	1.39	1.35
6	B	3003	FAD	C6-C7	2.44	1.44	1.37
6	B	3003	FAD	P-O1P	2.73	1.61	1.51
6	B	3003	FAD	C3B-C4B	2.78	1.60	1.53
6	A	2003	FAD	C10-N10	3.54	1.43	1.39
6	B	3003	FAD	C10-N10	3.54	1.43	1.39
6	B	3003	FAD	C5X-N5	4.16	1.42	1.35
6	A	2003	FAD	C5X-N5	4.48	1.42	1.35
6	B	3003	FAD	C10-N1	4.60	1.43	1.35
6	A	2003	FAD	C10-N1	5.00	1.43	1.35
6	B	3003	FAD	C4-N3	5.10	1.42	1.33
6	B	3003	FAD	C4X-N5	5.39	1.41	1.33
6	A	2003	FAD	C4-N3	5.66	1.43	1.33
6	A	2003	FAD	C4X-N5	5.71	1.42	1.33
6	B	3003	FAD	C9A-N10	5.79	1.46	1.38
6	A	2003	FAD	C9A-N10	5.81	1.46	1.38
6	A	2003	FAD	O4B-C1B	7.41	1.50	1.41
6	B	3003	FAD	O4B-C1B	9.36	1.53	1.41
6	B	3003	FAD	C2B-C3B	9.60	1.79	1.53

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	3003	FAD	N3A-C2A-N1A	-14.26	117.97	128.89
6	A	2003	FAD	N3A-C2A-N1A	-13.94	118.22	128.89
7	B	4002	URC	N7-C8-N9	-4.35	105.88	108.88
7	A	4001	URC	N7-C8-N9	-4.11	106.05	108.88
6	A	2003	FAD	O3P-PA-O5B	-3.01	94.96	102.94
6	A	2003	FAD	O4B-C4B-C3B	-2.68	99.76	105.15
6	A	2003	FAD	C4A-C5A-N7A	-2.37	107.30	109.48
6	B	3003	FAD	C4A-C5A-N7A	-2.26	107.40	109.48
6	A	2003	FAD	C4X-C10-N10	-2.22	119.21	120.52
6	A	2003	FAD	O2B-C2B-C3B	-2.21	104.63	111.83
6	B	3003	FAD	C4X-C10-N10	-2.15	119.25	120.52
6	A	2003	FAD	C4X-C4-N3	-2.12	120.68	123.59
6	B	3003	FAD	C4X-C4-N3	-2.03	120.81	123.59
6	A	2003	FAD	C6-C5X-C9A	2.19	121.86	118.98
6	A	2003	FAD	C5B-C4B-C3B	2.27	124.24	115.21
6	A	2003	FAD	C2A-N1A-C6A	2.29	122.85	118.77
6	B	3003	FAD	C6-C5X-C9A	2.31	122.02	118.98
6	B	3003	FAD	C2A-N1A-C6A	2.46	123.17	118.77
6	B	3003	FAD	P-O3P-PA	2.58	139.97	132.73
6	B	3003	FAD	C1'-C2'-C3'	2.78	117.77	109.82
6	A	2003	FAD	C1'-C2'-C3'	2.81	117.85	109.82
6	A	2003	FAD	C2B-C3B-C4B	2.97	108.72	102.61
6	B	3003	FAD	C5B-C4B-C3B	3.35	128.52	115.21
6	B	3003	FAD	O2P-P-O3P	3.56	121.27	105.09
7	A	4001	URC	N1-C2-N3	3.77	120.27	116.14
7	B	4002	URC	N1-C2-N3	3.79	120.29	116.14
6	A	2003	FAD	O3B-C3B-C2B	4.16	125.35	111.83
6	A	2003	FAD	C4X-N5-C5X	4.30	121.71	116.76
6	B	3003	FAD	C4X-N5-C5X	4.48	121.92	116.76
6	A	2003	FAD	C4-N3-C2	5.60	120.09	115.25
6	B	3003	FAD	C4-N3-C2	5.64	120.12	115.25
7	B	4002	URC	C5-C4-N9	5.75	105.24	102.69
7	A	4001	URC	C5-C4-N9	5.96	105.33	102.69
7	A	4001	URC	N9-C4-N3	10.52	132.49	112.36
7	B	4002	URC	N9-C4-N3	10.63	132.70	112.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2002	FES	1	0
6	A	2003	FAD	1	0
3	A	6002	PO4	1	0
5	B	2002	FES	1	0
6	B	3003	FAD	3	0
3	B	6003	PO4	1	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	1291/1331 (96%)	-0.08	61 (4%)	35	43	14, 29, 57, 96	0
1	B	1281/1331 (96%)	-0.11	46 (3%)	46	54	13, 26, 53, 116	0
All	All	2572/2662 (96%)	-0.10	107 (4%)	40	47	13, 28, 55, 116	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	553	PRO	12.3
1	A	1289	ALA	12.0
1	A	1288	ASN	10.8
1	B	554	PRO	8.6
1	B	1288	ASN	8.2
1	A	61	LEU	7.9
1	B	61	LEU	7.6
1	B	540	PRO	7.5
1	A	191	SER	7.0
1	B	541	THR	6.9
1	B	543	ALA	6.9
1	B	552	ASP	6.9
1	B	1289	ALA	6.7
1	B	191	SER	6.6
1	B	547	LEU	6.5
1	B	529	ALA	6.5
1	A	549	PHE	5.9
1	A	551	LYS	5.8
1	B	546	THR	5.7
1	A	550	GLN	5.5
1	B	1287	ASP	5.4
1	B	544	SER	4.9
1	A	221	THR	4.8
1	B	555	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	192	PRO	4.5
1	B	1320	VAL	4.5
1	A	95	GLN	4.4
1	B	63	ASN	4.4
1	B	1286	GLY	4.4
1	A	1290	LYS	4.4
1	B	527	GLY	4.4
1	A	165	ASP	4.4
1	B	165	ASP	4.2
1	B	1318	THR	4.1
1	A	1111	GLY	4.0
1	B	531	LEU	4.0
1	A	1287	ASP	3.9
1	B	530	ASP	3.9
1	B	542	PHE	3.9
1	A	552	ASP	3.6
1	A	386	HIS	3.6
1	A	250	GLN	3.5
1	A	1110	THR	3.5
1	B	220	ASP	3.4
1	A	423	ALA	3.4
1	B	528	ARG	3.2
1	B	565	LYS	3.1
1	A	1315	LEU	3.1
1	A	553	PRO	3.1
1	B	164	LYS	3.0
1	A	496	ALA	3.0
1	A	424	SER	3.0
1	A	1318	THR	3.0
1	A	1316	CYS	2.9
1	A	529	ALA	2.8
1	B	1143	GLU	2.8
1	B	222	PRO	2.8
1	A	497	PRO	2.8
1	A	428	ASP	2.7
1	A	474	SER	2.7
1	A	566	ASP	2.7
1	B	334	ARG	2.7
1	A	292	GLY	2.7
1	B	1111	GLY	2.7
1	A	271	ASN	2.7
1	A	467	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	537	LYS	2.6
1	B	474	SER	2.5
1	B	1108	LYS	2.5
1	B	95	GLN	2.5
1	A	720	LYS	2.4
1	A	1143	GLU	2.4
1	A	220	ASP	2.4
1	A	193	SER	2.4
1	B	386	HIS	2.3
1	A	3	ALA	2.3
1	A	1286	GLY	2.3
1	B	480	GLU	2.3
1	A	686	LYS	2.3
1	B	317	LYS	2.3
1	B	219	LYS	2.3
1	B	288	SER	2.2
1	A	466	LEU	2.2
1	A	320	GLU	2.2
1	A	532	GLU	2.2
1	B	566	ASP	2.2
1	B	221	THR	2.2
1	A	534	MET	2.2
1	A	498	ASP	2.1
1	A	63	ASN	2.1
1	A	565	LYS	2.1
1	A	60	ARG	2.1
1	A	1107	LYS	2.1
1	A	699	GLN	2.1
1	B	526	LEU	2.1
1	A	321	GLN	2.1
1	A	693	PRO	2.1
1	A	334	ARG	2.0
1	A	218	LEU	2.0
1	A	392	TYR	2.0
1	A	64	LYS	2.0
1	A	222	PRO	2.0
1	A	293	PRO	2.0
1	A	461	ARG	2.0
1	B	972	ILE	2.0
1	A	387	THR	2.0
1	B	982	ARG	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
3	PO4	A	6006	5/5	0.95	0.25	2.04	80,80,81,81	0
3	PO4	B	6007	5/5	0.96	0.16	1.74	72,72,73,73	0
3	PO4	B	6010	5/5	0.94	0.20	1.54	69,70,71,71	0
3	PO4	B	6011	5/5	0.98	0.20	1.47	49,50,51,53	0
7	URC	B	4002	12/12	0.93	0.12	1.39	32,34,39,39	0
3	PO4	B	6005	5/5	0.91	0.19	1.32	82,83,84,84	0
3	PO4	A	6004	5/5	0.78	0.23	0.99	97,97,98,99	0
2	BCT	B	5002	4/4	0.99	0.12	0.40	22,22,23,24	0
7	URC	A	4001	12/12	0.95	0.10	0.35	31,34,35,38	0
3	PO4	B	6003	5/5	0.98	0.11	0.07	32,33,39,40	0
3	PO4	A	6008	5/5	0.94	0.13	-0.10	73,74,74,75	0
3	PO4	A	6002	5/5	0.98	0.10	-0.54	34,37,39,42	0
6	FAD	A	2003	53/53	0.97	0.09	-0.77	20,28,31,37	0
6	FAD	B	3003	53/53	0.98	0.09	-0.92	14,22,26,28	0
2	BCT	A	5001	4/4	0.99	0.09	-1.10	23,25,25,26	0
4	CA	B	7004	1/1	0.99	0.06	-1.16	22,22,22,22	0
5	FES	A	2001	4/4	0.96	0.07	-1.79	31,32,32,34	0
5	FES	B	2002	4/4	0.99	0.06	-1.92	19,20,20,21	0
5	FES	B	2001	4/4	0.96	0.07	-2.13	26,30,30,33	0
4	CA	B	7001	1/1	0.99	0.07	-2.33	21,21,21,21	0
4	CA	A	7003	1/1	0.99	0.03	-2.78	22,22,22,22	0
5	FES	A	2002	4/4	0.99	0.05	-2.91	20,20,21,21	0
4	CA	A	7002	1/1	1.00	0.07	-3.01	23,23,23,23	0
3	PO4	A	6001	5/5	0.95	0.20	-	46,48,51,51	0
3	PO4	A	6009	5/5	0.90	0.27	-	85,86,86,87	0

6.5 Other polymers (i)

There are no such residues in this entry.