Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:17 PM GMT

PDB ID	:	4EAZ
Title	:	Vgll1-TEAD4 structure
Authors	:	Pobbati, A.V.; Song, H.
Deposited on	:	2012-03-23
Resolution	:	2.80 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:

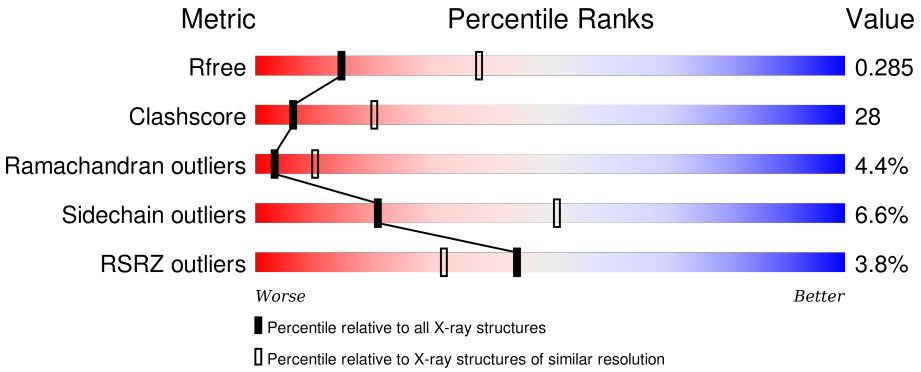
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	C	60	5% 37% 13% 5% 45%
1	D	60	25% 25% • 47%
2	A	223	4% 62% 31% • •
2	B	223	3% 52% 36% 6% • •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4086 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 Transcription cofactor vestigial-like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	33	Total	C	N	O	Se	0	0	0
			270	171	46	52	1			
1	D	32	Total	C	N	O	Se	0	0	0
			262	167	44	50	1			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	6	MSE	-	EXPRESSION TAG	UNP Q99NC0
C	7	GLY	-	EXPRESSION TAG	UNP Q99NC0
C	8	SER	-	EXPRESSION TAG	UNP Q99NC0
C	9	SER	-	EXPRESSION TAG	UNP Q99NC0
C	10	HIS	-	EXPRESSION TAG	UNP Q99NC0
C	11	HIS	-	EXPRESSION TAG	UNP Q99NC0
C	12	HIS	-	EXPRESSION TAG	UNP Q99NC0
C	13	HIS	-	EXPRESSION TAG	UNP Q99NC0
C	14	HIS	-	EXPRESSION TAG	UNP Q99NC0
C	15	HIS	-	EXPRESSION TAG	UNP Q99NC0
C	16	SER	-	EXPRESSION TAG	UNP Q99NC0
C	17	GLN	-	EXPRESSION TAG	UNP Q99NC0
C	18	ASP	-	EXPRESSION TAG	UNP Q99NC0
C	19	PRO	-	EXPRESSION TAG	UNP Q99NC0
C	52	MSE	-	EXPRESSION TAG	UNP Q99NC0
C	53	GLY	-	EXPRESSION TAG	UNP Q99NC0
C	54	SER	-	EXPRESSION TAG	UNP Q99NC0
C	55	SER	-	EXPRESSION TAG	UNP Q99NC0
C	56	HIS	-	EXPRESSION TAG	UNP Q99NC0
C	57	HIS	-	EXPRESSION TAG	UNP Q99NC0
C	58	HIS	-	EXPRESSION TAG	UNP Q99NC0
C	59	HIS	-	EXPRESSION TAG	UNP Q99NC0
C	60	HIS	-	EXPRESSION TAG	UNP Q99NC0
C	61	HIS	-	EXPRESSION TAG	UNP Q99NC0
C	62	SER	-	EXPRESSION TAG	UNP Q99NC0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	63	GLN	-	EXPRESSION TAG	UNP Q99NC0
C	64	ASP	-	EXPRESSION TAG	UNP Q99NC0
C	65	PRO	-	EXPRESSION TAG	UNP Q99NC0
D	6	MSE	-	EXPRESSION TAG	UNP Q99NC0
D	7	GLY	-	EXPRESSION TAG	UNP Q99NC0
D	8	SER	-	EXPRESSION TAG	UNP Q99NC0
D	9	SER	-	EXPRESSION TAG	UNP Q99NC0
D	10	HIS	-	EXPRESSION TAG	UNP Q99NC0
D	11	HIS	-	EXPRESSION TAG	UNP Q99NC0
D	12	HIS	-	EXPRESSION TAG	UNP Q99NC0
D	13	HIS	-	EXPRESSION TAG	UNP Q99NC0
D	14	HIS	-	EXPRESSION TAG	UNP Q99NC0
D	15	HIS	-	EXPRESSION TAG	UNP Q99NC0
D	16	SER	-	EXPRESSION TAG	UNP Q99NC0
D	17	GLN	-	EXPRESSION TAG	UNP Q99NC0
D	18	ASP	-	EXPRESSION TAG	UNP Q99NC0
D	19	PRO	-	EXPRESSION TAG	UNP Q99NC0
D	52	MSE	-	EXPRESSION TAG	UNP Q99NC0
D	53	GLY	-	EXPRESSION TAG	UNP Q99NC0
D	54	SER	-	EXPRESSION TAG	UNP Q99NC0
D	55	SER	-	EXPRESSION TAG	UNP Q99NC0
D	56	HIS	-	EXPRESSION TAG	UNP Q99NC0
D	57	HIS	-	EXPRESSION TAG	UNP Q99NC0
D	58	HIS	-	EXPRESSION TAG	UNP Q99NC0
D	59	HIS	-	EXPRESSION TAG	UNP Q99NC0
D	60	HIS	-	EXPRESSION TAG	UNP Q99NC0
D	61	HIS	-	EXPRESSION TAG	UNP Q99NC0
D	62	SER	-	EXPRESSION TAG	UNP Q99NC0
D	63	GLN	-	EXPRESSION TAG	UNP Q99NC0
D	64	ASP	-	EXPRESSION TAG	UNP Q99NC0
D	65	PRO	-	EXPRESSION TAG	UNP Q99NC0

- Molecule 2 is a protein called Transcriptional enhancer factor TEF-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	218	Total	C	N	O	S	0	0	0
			1796	1152	298	336	10			
2	B	213	Total	C	N	O	S	0	0	0
			1755	1127	292	326	10			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	205	ASP	-	EXPRESSION TAG	UNP Q62296
A	206	PRO	-	EXPRESSION TAG	UNP Q62296
A	207	ASN	-	EXPRESSION TAG	UNP Q62296
A	208	SER	-	EXPRESSION TAG	UNP Q62296
A	209	MET	-	EXPRESSION TAG	UNP Q62296
B	205	ASP	-	EXPRESSION TAG	UNP Q62296
B	206	PRO	-	EXPRESSION TAG	UNP Q62296
B	207	ASN	-	EXPRESSION TAG	UNP Q62296
B	208	SER	-	EXPRESSION TAG	UNP Q62296
B	209	MET	-	EXPRESSION TAG	UNP Q62296

- Molecule 3 is water.

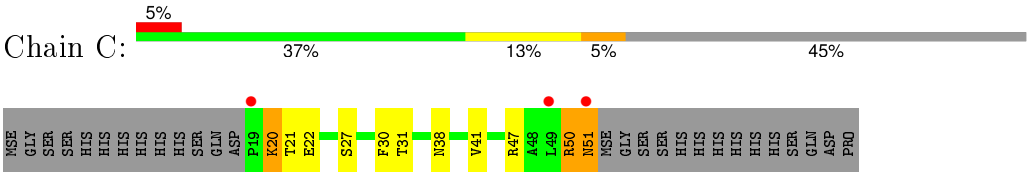
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total O 2 2	0	0
3	B	1	Total O 1 1	0	0

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.

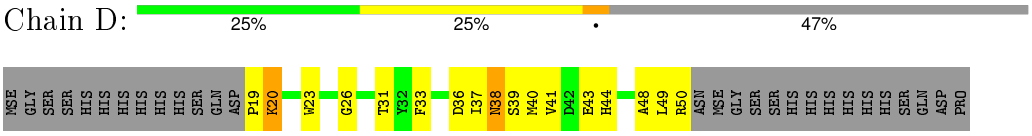
- Molecule 1: Transcription cofactor vestigial-like protein 1

Chain C:



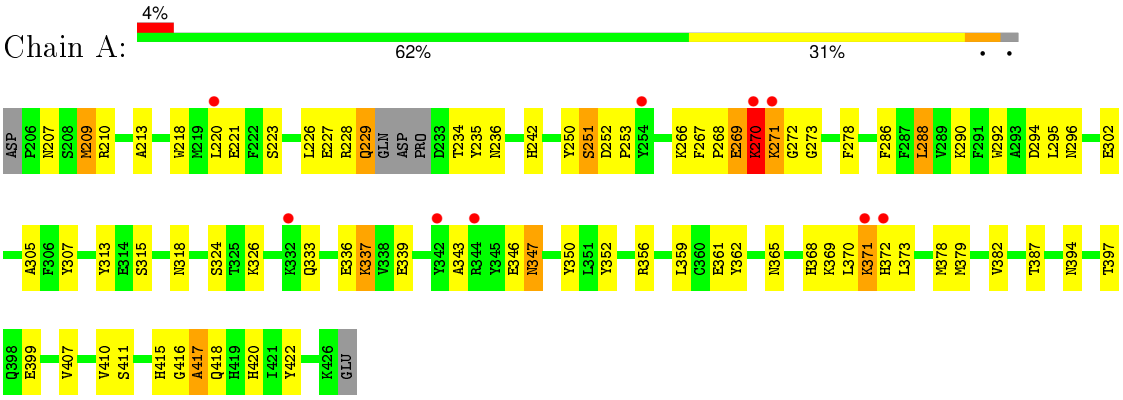
- Molecule 1: Transcription cofactor vestigial-like protein 1

Chain D:



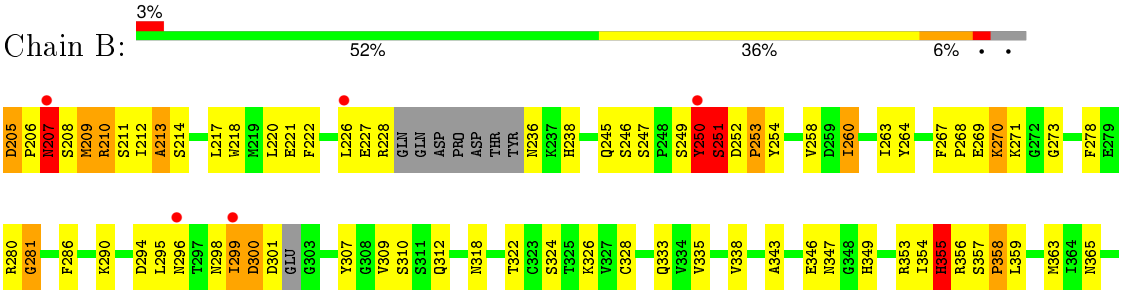
- Molecule 2: Transcriptional enhancer factor TEF-3

Chain A:



- Molecule 2: Transcriptional enhancer factor TEF-3

Chain B:




H368
K369
L370
K371
H372
T387
I388
R395
D396
T397
Q398
E399
L402
A405
Y406
V407
F408
E409
V410
S411
A412
S413
E414
H415
GLY
A417
H420
I421
Y422
R423
K426
GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	113.93Å 113.93Å 144.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	58.26 – 2.80 98.67 – 2.74	Depositor EDS
% Data completeness (in resolution range)	96.3 (58.26-2.80) 94.6 (98.67-2.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 2.73Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.211 , 0.272 0.235 , 0.285	Depositor DCC
R_{free} test set	1321 reflections (5.04%)	DCC
Wilson B-factor (Å^2)	73.7	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 62.7	EDS
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 28983 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4086	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% 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

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	C	0.43	0/276	0.55	0/370
1	D	0.40	0/268	0.52	0/359
2	A	0.44	0/1842	0.62	0/2487
2	B	0.43	0/1798	0.58	1/2425 (0.0%)
All	All	0.44	0/4184	0.59	1/5641 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	205	ASP	C-N-CD	-5.37	108.79	120.60

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	C	270	0	248	10	0
1	D	262	0	242	14	0
2	A	1796	0	1741	95	0
2	B	1755	0	1705	117	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
All	All	4086	0	3936	222	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 28.

All (222) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:205:ASP:HB3	2:B:206:PRO:CD	1.46	1.43
2:B:205:ASP:CB	2:B:206:PRO:HD3	1.57	1.28
2:A:368:HIS:CE1	2:A:372:HIS:HE1	1.58	1.21
2:B:209:MET:CE	2:B:254:TYR:HE1	1.55	1.19
2:B:209:MET:CE	2:B:254:TYR:CE1	2.26	1.19
2:A:294:ASP:CB	2:A:416:GLY:O	1.93	1.16
2:B:209:MET:HE1	2:B:254:TYR:CE1	1.80	1.15
2:A:242:HIS:HB2	2:B:250:TYR:OH	1.46	1.14
2:A:294:ASP:HB2	2:A:416:GLY:O	0.98	1.14
2:A:368:HIS:CE1	2:A:372:HIS:CE1	2.36	1.13
2:A:250:TYR:HA	2:A:251:SER:C	1.71	1.08
2:B:268:PRO:O	2:B:273:GLY:HA2	1.55	1.06
2:B:213:ALA:CB	2:B:218:TRP:HA	1.88	1.03
2:A:295:LEU:O	2:A:371:LYS:CD	2.12	0.98
2:B:210:ARG:HD3	2:B:252:ASP:HB2	1.45	0.98
2:B:213:ALA:HB2	2:B:218:TRP:HA	1.43	0.97
2:A:296:ASN:ND2	2:A:415:HIS:CE1	2.33	0.96
2:B:209:MET:HE1	2:B:254:TYR:HE1	1.17	0.95
2:B:209:MET:HE2	2:B:254:TYR:CD1	2.03	0.94
2:B:205:ASP:HB3	2:B:206:PRO:HD3	0.92	0.92
2:A:252:ASP:HB3	2:A:253:PRO:HD2	1.48	0.92
2:B:205:ASP:CB	2:B:206:PRO:CD	2.28	0.91
2:A:295:LEU:O	2:A:371:LYS:HD3	1.68	0.90
2:B:205:ASP:HB3	2:B:206:PRO:HD2	1.49	0.90
2:B:354:ILE:HG22	2:B:354:ILE:O	1.72	0.87
2:B:310:SER:HA	2:B:355:HIS:O	1.75	0.85
2:A:295:LEU:HB3	2:A:371:LYS:HG3	1.59	0.84
2:B:209:MET:CE	2:B:254:TYR:CD1	2.60	0.83
2:B:210:ARG:HB3	2:B:252:ASP:HB3	1.59	0.83
2:B:269:GLU:O	2:B:270:LYS:HB2	1.78	0.83
2:A:223:SER:HB3	2:B:250:TYR:CZ	2.14	0.83
2:B:209:MET:HE2	2:B:254:TYR:CE1	2.16	0.80
2:A:229:GLN:HG2	2:A:229:GLN:O	1.82	0.80
2:A:296:ASN:HD21	2:A:415:HIS:CE1	1.96	0.79
2:B:213:ALA:HB1	2:B:217:LEU:O	1.81	0.79
2:A:373:LEU:HD12	2:A:379:MET:HA	1.63	0.79
2:B:213:ALA:HB1	2:B:218:TRP:HA	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:223:SER:HB3	2:B:250:TYR:CE1	2.20	0.77
2:B:268:PRO:HD3	2:B:328:CYS:SG	2.26	0.76
2:A:373:LEU:HD12	2:A:379:MET:CA	2.16	0.75
2:B:210:ARG:HD3	2:B:252:ASP:CB	2.15	0.75
2:A:210:ARG:HD3	2:A:252:ASP:O	1.87	0.74
1:C:50:ARG:HA	1:C:51:ASN:C	2.07	0.74
2:B:267:PHE:HB3	2:B:268:PRO:HD2	1.70	0.73
2:B:209:MET:SD	2:B:254:TYR:HE1	2.10	0.73
2:A:379:MET:SD	2:A:410:VAL:HG21	2.30	0.71
2:B:299:ILE:O	2:B:301:ASP:N	2.22	0.71
2:B:205:ASP:CG	2:B:206:PRO:HD3	2.11	0.71
2:B:209:MET:HE2	2:B:254:TYR:HD1	1.51	0.71
2:A:368:HIS:NE2	2:A:372:HIS:HE1	1.89	0.70
2:B:354:ILE:CG2	2:B:354:ILE:O	2.40	0.70
2:B:238:HIS:HE1	2:B:294:ASP:O	1.76	0.69
2:A:242:HIS:HB2	2:B:250:TYR:CZ	2.28	0.68
2:B:395:ARG:HG2	2:B:395:ARG:NH1	2.09	0.68
2:A:346:GLU:O	2:A:347:ASN:HB2	1.92	0.67
2:B:206:PRO:C	2:B:208:SER:H	1.96	0.67
2:B:395:ARG:HG2	2:B:395:ARG:HH11	1.59	0.67
2:B:309:VAL:O	2:B:356:ARG:HA	1.95	0.67
2:A:318:ASN:HB2	2:A:350:TYR:CZ	2.31	0.66
2:A:416:GLY:O	2:A:417:ALA:HB2	1.96	0.65
2:B:208:SER:C	2:B:210:ARG:H	2.00	0.65
2:A:250:TYR:HA	2:A:251:SER:O	1.95	0.65
2:A:210:ARG:CD	2:A:252:ASP:O	2.44	0.65
2:B:271:LYS:C	2:B:273:GLY:H	2.00	0.65
2:B:298:ASN:O	2:B:299:ILE:C	2.35	0.65
2:A:343:ALA:HB2	2:A:352:TYR:CE1	2.31	0.65
2:B:206:PRO:O	2:B:208:SER:N	2.30	0.64
2:B:250:TYR:O	2:B:252:ASP:N	2.30	0.64
2:A:242:HIS:CB	2:B:250:TYR:OH	2.37	0.64
1:D:23:TRP:CH2	1:D:26:GLY:HA2	2.32	0.64
2:A:226:LEU:HD11	2:A:305:ALA:HB1	1.80	0.64
2:A:271:LYS:O	2:A:273:GLY:N	2.30	0.63
2:A:278:PHE:HA	2:A:286:PHE:CZ	2.34	0.63
2:B:249:SER:O	2:B:250:TYR:C	2.37	0.63
2:B:298:ASN:O	2:B:300:ASP:N	2.32	0.63
1:C:47:ARG:O	1:C:47:ARG:HG2	1.97	0.63
2:A:418:GLN:N	2:A:418:GLN:CD	2.53	0.62
2:A:226:LEU:HG	2:A:226:LEU:O	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:296:ASN:ND2	2:B:415:HIS:CE1	2.68	0.62
2:B:212:ILE:O	2:B:213:ALA:HB2	1.99	0.61
2:A:296:ASN:HD21	2:A:415:HIS:HE1	1.43	0.61
2:A:295:LEU:O	2:A:371:LYS:HD2	1.99	0.60
2:B:210:ARG:CB	2:B:252:ASP:HB3	2.28	0.60
2:A:397:THR:O	2:A:399:GLU:N	2.34	0.60
2:A:369:LYS:O	2:A:372:HIS:HB2	2.02	0.60
2:A:207:ASN:O	2:A:209:MET:N	2.34	0.60
2:A:373:LEU:CD1	2:A:379:MET:HA	2.31	0.60
2:B:269:GLU:HA	2:B:273:GLY:HA3	1.84	0.59
2:A:228:ARG:NH2	2:A:302:GLU:OE1	2.35	0.59
2:A:296:ASN:HD22	2:A:415:HIS:CE1	2.21	0.58
2:A:229:GLN:O	2:A:229:GLN:CG	2.49	0.58
2:A:318:ASN:HB2	2:A:350:TYR:CE1	2.38	0.58
2:B:318:ASN:OD1	2:B:343:ALA:HB3	2.03	0.58
2:B:264:TYR:HB3	2:B:269:GLU:OE2	2.04	0.58
2:B:397:THR:O	2:B:398:GLN:C	2.42	0.58
2:A:251:SER:HB3	2:A:252:ASP:O	2.04	0.58
2:A:296:ASN:ND2	2:A:415:HIS:ND1	2.52	0.57
2:A:221:GLU:HG3	2:B:250:TYR:CE1	2.39	0.57
2:B:258:VAL:HG11	2:B:263:ILE:HD11	1.86	0.56
2:A:269:GLU:O	2:A:270:LYS:C	2.45	0.55
2:B:295:LEU:HD11	2:B:370:LEU:HD23	1.89	0.55
2:B:209:MET:SD	2:B:254:TYR:CE1	2.94	0.55
2:A:410:VAL:HG12	2:A:411:SER:O	2.07	0.55
1:C:41:VAL:HG11	2:B:365:ASN:ND2	2.22	0.55
2:A:252:ASP:HB3	2:A:253:PRO:CD	2.29	0.55
2:B:249:SER:O	2:B:251:SER:N	2.40	0.54
1:D:41:VAL:HG21	2:A:365:ASN:HD22	1.72	0.54
2:A:210:ARG:HD2	2:A:252:ASP:N	2.23	0.54
1:C:51:ASN:OD1	1:C:51:ASN:N	2.40	0.53
2:B:326:LYS:HD3	2:B:333:GLN:HE21	1.73	0.53
2:B:208:SER:O	2:B:210:ARG:N	2.41	0.53
1:C:41:VAL:HG11	2:B:365:ASN:HD22	1.73	0.53
1:D:37:ILE:HG21	2:A:362:TYR:HA	1.91	0.52
1:C:20:LYS:HB3	1:C:31:THR:OG1	2.08	0.52
2:B:290:LYS:HZ1	2:B:409:GLU:CD	2.13	0.52
2:B:206:PRO:C	2:B:208:SER:N	2.63	0.52
2:A:290:LYS:HD3	2:A:292:TRP:CH2	2.45	0.51
1:D:49:LEU:O	1:D:50:ARG:C	2.49	0.51
2:B:395:ARG:CG	2:B:395:ARG:HH11	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:210:ARG:CD	2:B:252:ASP:HB2	2.28	0.51
2:B:252:ASP:O	2:B:253:PRO:C	2.49	0.51
2:A:373:LEU:HD12	2:A:379:MET:N	2.26	0.50
2:B:357:SER:O	2:B:358:PRO:C	2.49	0.50
1:D:19:PRO:O	1:D:20:LYS:O	2.30	0.50
2:B:227:GLU:OE1	2:B:356:ARG:NH1	2.45	0.49
2:B:251:SER:O	2:B:252:ASP:OD2	2.30	0.49
2:A:373:LEU:CD1	2:A:379:MET:N	2.75	0.49
1:C:20:LYS:O	1:C:30:PHE:HA	2.12	0.49
2:A:266:LYS:HB3	2:A:387:THR:HG21	1.93	0.49
2:A:267:PHE:HB3	2:A:268:PRO:HD2	1.94	0.49
2:A:394:ASN:HB3	2:A:397:THR:O	2.13	0.49
2:B:213:ALA:HB1	2:B:218:TRP:CA	2.36	0.49
2:B:324:SER:HB2	2:B:338:VAL:HG22	1.94	0.49
2:B:207:ASN:OD1	2:B:207:ASN:O	2.30	0.49
1:D:36:ASP:OD2	1:D:36:ASP:C	2.50	0.49
2:B:221:GLU:HG2	2:B:222:PHE:N	2.28	0.49
2:B:309:VAL:HG13	2:B:357:SER:OG	2.13	0.49
2:A:226:LEU:HD13	2:A:307:TYR:CZ	2.48	0.49
2:B:354:ILE:O	2:B:355:HIS:C	2.51	0.48
2:B:238:HIS:CE1	2:B:294:ASP:O	2.63	0.48
2:B:278:PHE:HA	2:B:286:PHE:CZ	2.47	0.48
2:B:299:ILE:O	2:B:300:ASP:C	2.51	0.48
2:B:397:THR:O	2:B:399:GLU:N	2.46	0.48
2:B:299:ILE:C	2:B:301:ASP:N	2.65	0.48
1:D:33:PHE:HB3	1:D:40:MSE:HE2	1.96	0.48
2:B:294:ASP:HB2	2:B:417:ALA:HB2	1.95	0.48
2:B:208:SER:C	2:B:210:ARG:N	2.66	0.47
2:B:299:ILE:C	2:B:301:ASP:H	2.17	0.47
2:B:246:SER:O	2:B:247:SER:C	2.52	0.47
1:C:20:LYS:HB2	1:C:31:THR:O	2.14	0.47
2:A:420:HIS:ND1	2:A:422:TYR:CZ	2.81	0.47
2:A:270:LYS:HB3	2:A:271:LYS:H	1.50	0.47
2:B:260:ILE:HG12	2:B:264:TYR:CE1	2.50	0.47
1:D:36:ASP:OD2	1:D:36:ASP:O	2.33	0.47
2:A:210:ARG:NE	2:A:251:SER:O	2.48	0.46
2:A:234:THR:O	2:A:235:TYR:HB2	2.15	0.46
1:C:41:VAL:HG21	2:B:365:ASN:HD22	1.79	0.46
2:B:222:PHE:C	2:B:222:PHE:CD2	2.88	0.46
2:B:210:ARG:HH11	2:B:210:ARG:HG3	1.81	0.46
2:B:271:LYS:C	2:B:273:GLY:N	2.66	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:226:LEU:HD13	2:B:307:TYR:CZ	2.50	0.46
2:A:294:ASP:HB2	2:A:417:ALA:HB2	1.96	0.46
2:A:295:LEU:O	2:A:371:LYS:CG	2.64	0.46
1:D:37:ILE:O	1:D:38:ASN:C	2.52	0.46
2:A:226:LEU:CD1	2:A:305:ALA:HB1	2.44	0.46
2:B:267:PHE:CZ	2:B:405:ALA:HB1	2.51	0.46
2:B:212:ILE:O	2:B:213:ALA:CB	2.64	0.46
1:D:19:PRO:O	1:D:31:THR:O	2.33	0.45
2:A:213:ALA:HB2	2:A:218:TRP:HD1	1.81	0.45
1:D:39:SER:O	1:D:43:GLU:HB2	2.16	0.45
2:A:227:GLU:CD	2:A:356:ARG:HH12	2.17	0.45
2:A:326:LYS:HD3	2:A:333:GLN:HE21	1.81	0.45
2:B:228:ARG:HD2	2:B:228:ARG:HA	1.66	0.45
2:B:213:ALA:HA	2:B:402:LEU:HD21	1.99	0.45
2:A:371:LYS:HE3	2:A:371:LYS:HB3	1.53	0.45
2:A:223:SER:CB	2:B:250:TYR:CE1	2.97	0.45
2:A:337:LYS:HD3	2:A:339:GLU:OE2	2.17	0.45
2:B:296:ASN:HD22	2:B:415:HIS:CE1	2.33	0.45
1:D:33:PHE:CG	1:D:40:MSE:HG2	2.52	0.45
2:B:280:ARG:CG	2:B:281:GLY:N	2.80	0.44
2:B:210:ARG:HH11	2:B:210:ARG:CG	2.29	0.44
2:A:368:HIS:O	2:A:372:HIS:ND1	2.50	0.44
2:A:251:SER:HB3	2:A:252:ASP:C	2.37	0.44
2:B:420:HIS:ND1	2:B:422:TYR:CZ	2.85	0.44
2:B:368:HIS:NE2	2:B:372:HIS:HE1	2.15	0.44
2:A:416:GLY:O	2:A:417:ALA:CB	2.61	0.44
2:B:269:GLU:HA	2:B:273:GLY:CA	2.46	0.44
2:A:218:TRP:CZ3	2:A:220:LEU:HB2	2.52	0.44
2:B:211:SER:HB2	2:B:245:GLN:OE1	2.17	0.44
1:C:21:THR:HG22	1:C:22:GLU:N	2.32	0.44
2:A:210:ARG:HB3	2:A:253:PRO:O	2.19	0.43
2:B:328:CYS:HB2	2:B:387:THR:OG1	2.18	0.43
2:A:315:SER:HB3	2:A:352:TYR:HE2	1.82	0.43
2:A:292:TRP:O	2:A:417:ALA:HB1	2.19	0.43
2:A:313:TYR:N	2:A:313:TYR:CD2	2.85	0.43
2:A:220:LEU:O	2:A:220:LEU:HD12	2.19	0.43
2:B:226:LEU:HD13	2:B:307:TYR:CE2	2.53	0.43
2:A:228:ARG:NH1	2:A:236:ASN:OD1	2.51	0.43
2:B:423:ARG:HH11	2:B:423:ARG:HG3	1.83	0.43
2:A:343:ALA:HB2	2:A:352:TYR:CZ	2.54	0.42
2:A:270:LYS:HA	2:A:270:LYS:HD3	1.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:210:ARG:HD2	2:A:252:ASP:H	1.82	0.42
2:A:221:GLU:OE1	2:B:250:TYR:HD1	2.02	0.42
2:A:373:LEU:HD13	2:A:378:MET:C	2.40	0.42
2:B:346:GLU:O	2:B:349:HIS:CD2	2.72	0.42
2:B:309:VAL:CG1	2:B:357:SER:OG	2.66	0.42
2:B:220:LEU:HB3	2:B:312:GLN:HB2	2.00	0.42
2:B:359:LEU:HD21	2:B:363:MET:HB3	2.02	0.42
2:A:288:LEU:HD23	2:A:422:TYR:CD2	2.55	0.42
2:A:269:GLU:HB2	2:A:270:LYS:H	1.52	0.41
2:A:370:LEU:C	2:A:372:HIS:H	2.24	0.41
2:A:324:SER:OG	2:A:336:GLU:OE2	2.33	0.41
2:B:410:VAL:HG12	2:B:411:SER:N	2.36	0.41
2:A:326:LYS:HB2	2:A:326:LYS:HE3	1.90	0.41
2:A:361:GLU:HG2	2:A:361:GLU:O	2.21	0.40
2:B:263:ILE:CG2	2:B:267:PHE:HE2	2.34	0.40
2:B:253:PRO:O	2:B:254:TYR:C	2.60	0.40
2:A:269:GLU:O	2:A:273:GLY:HA3	2.22	0.40
1:D:44:HIS:CD2	1:D:44:HIS:C	2.94	0.40
2:B:296:ASN:ND2	2:B:415:HIS:HE1	2.19	0.40
1:D:48:ALA:HB1	2:A:382:VAL:HA	2.04	0.40
2:B:413:SER:O	2:B:414:GLU:C	2.60	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	C	31/60 (52%)	29 (94%)	2 (6%)	0	100 100
1	D	30/60 (50%)	25 (83%)	4 (13%)	1 (3%)	5 16
2	A	214/223 (96%)	196 (92%)	13 (6%)	5 (2%)	8 26
2	B	205/223 (92%)	177 (86%)	13 (6%)	15 (7%)	1 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	480/566 (85%)	427 (89%)	32 (7%)	21 (4%)	3 10

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	20	LYS
2	A	271	LYS
2	B	207	ASN
2	B	250	TYR
2	B	251	SER
2	B	299	ILE
2	B	300	ASP
2	A	270	LYS
2	A	272	GLY
2	A	417	ALA
2	B	209	MET
2	B	213	ALA
2	B	270	LYS
2	B	355	HIS
2	B	398	GLN
2	A	347	ASN
2	B	214	SER
2	B	347	ASN
2	B	253	PRO
2	B	358	PRO
2	B	281	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	C	29/51 (57%)	24 (83%)	5 (17%)	2 7
1	D	28/51 (55%)	27 (96%)	1 (4%)	42 76
2	A	201/206 (98%)	191 (95%)	10 (5%)	30 64
2	B	197/206 (96%)	183 (93%)	14 (7%)	18 46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	455/514 (88%)	425 (93%)	30 (7%)	21 51

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	20	LYS
1	C	27	SER
1	C	38	ASN
1	C	50	ARG
1	C	51	ASN
1	D	38	ASN
2	A	209	MET
2	A	229	GLN
2	A	251	SER
2	A	269	GLU
2	A	270	LYS
2	A	288	LEU
2	A	337	LYS
2	A	359	LEU
2	A	371	LYS
2	A	407	VAL
2	B	207	ASN
2	B	210	ARG
2	B	236	ASN
2	B	250	TYR
2	B	251	SER
2	B	260	ILE
2	B	322	THR
2	B	335	VAL
2	B	353	ARG
2	B	355	HIS
2	B	388	ILE
2	B	395	ARG
2	B	407	VAL
2	B	423	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	38	ASN
2	A	296	ASN

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Mol	Chain	Res	Type
2	A	333	GLN
2	A	365	ASN
2	A	368	HIS
2	A	372	HIS
2	A	415	HIS
2	A	418	GLN
2	B	238	HIS
2	B	296	ASN
2	B	333	GLN
2	B	365	ASN
2	B	372	HIS
2	B	415	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

There are no ligands in this entry.

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	C	32/60 (53%)	0.54	3 (9%) 11 5	61, 75, 112, 130	0
1	D	31/60 (51%)	0.46	0 100 100	60, 74, 100, 112	0
2	A	218/223 (97%)	0.52	9 (4%) 41 29	50, 80, 124, 153	0
2	B	213/223 (95%)	0.62	7 (3%) 50 38	51, 72, 122, 154	0
All	All	494/566 (87%)	0.56	19 (3%) 44 32	50, 76, 122, 154	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	250	TYR	5.6
2	A	254	TYR	3.4
2	B	415	HIS	3.3
2	B	226	LEU	3.1
2	A	270	LYS	3.0
2	A	344	ARG	2.8
2	B	207	ASN	2.7
1	C	51	ASN	2.7
2	B	398	GLN	2.6
2	B	296	ASN	2.6
2	A	332	LYS	2.5
2	A	271	LYS	2.5
1	C	49	LEU	2.3
2	A	372	HIS	2.3
2	B	299	ILE	2.2
2	A	371	LYS	2.2
2	A	342	TYR	2.2
2	A	220	LEU	2.0
1	C	19	PRO	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.