Preliminary Full wwPDB X-ray Structure Validation Report (i)

May 29, 2023 – 04:40 PM JST

Deposition ID : D_1300037952

This wwPDB validation report is NOT for manuscript review

This is a Preliminary Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB Deposition System
during initial deposition but before annotation of the structure.

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 (i)) were used in the production of this report:

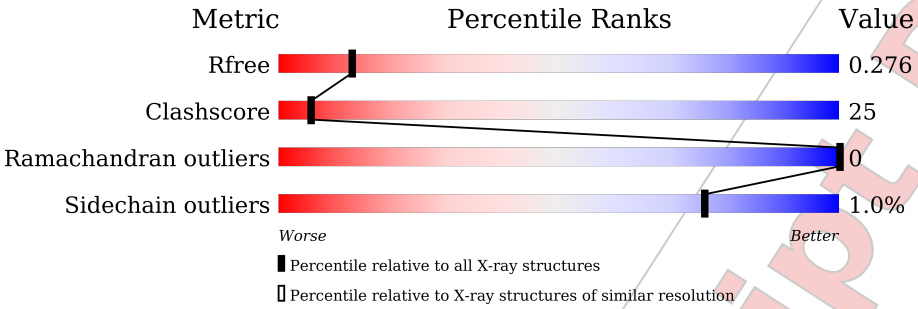
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.33
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

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 unknown.

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	-
Clashscore	141614	-
Ramachandran outliers	138981	-
Sidechain outliers	138945	-

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%

Mol	Chain	Length	Quality of chain
1	A	296	54% 44% .
2	B	299	61% 38% .
3	C	21	57% 38% 5%
4	D	20	60% 35% 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5360 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	296	2428	1553	417	445	13	0	0	0

- Molecule 2 is a protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	299	2460	1577	421	449	13	0	0	0

- Molecule 3 is a protein called ARG-HIS-VAL-SER-SER-SER-ASP-ARG-VAL-GLY-LYS-PRO-TYR-ARG-GLY-VAL-LYS-PRO-VAL-PHE-SER.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	21	166	104	34	28	0	0	0

- Molecule 4 is a protein called ARG-HIS-VAL-SER-SER-SER-ASP-ARG-VAL-GLY-LYS-PRO-TYR-ARG-GLY-VAL-LYS-PRO-VAL-PHE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	D	20	160	101	33	26	0	0	0

- Molecule 5 is water.

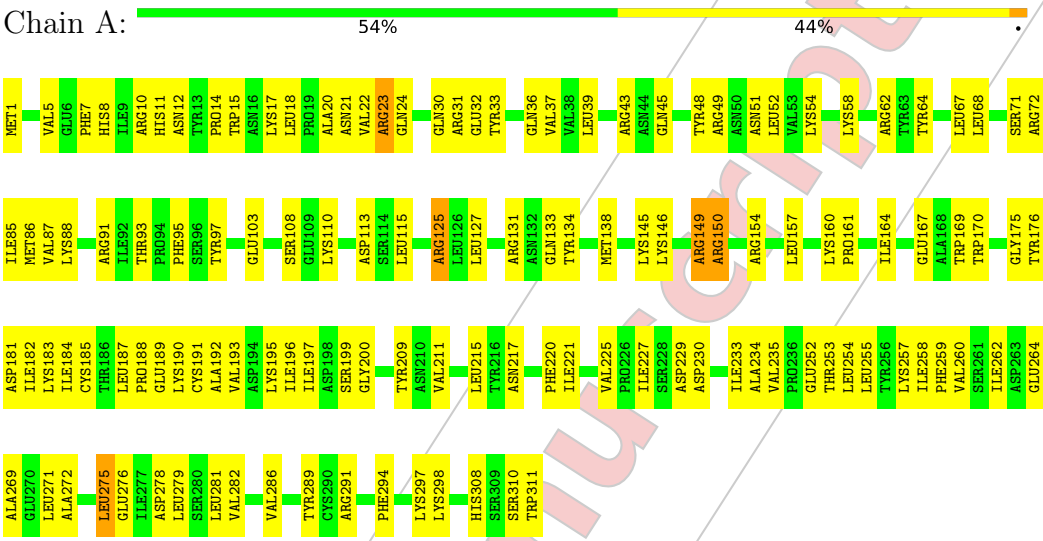
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	S	146	146	146	0	0

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. 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. 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.

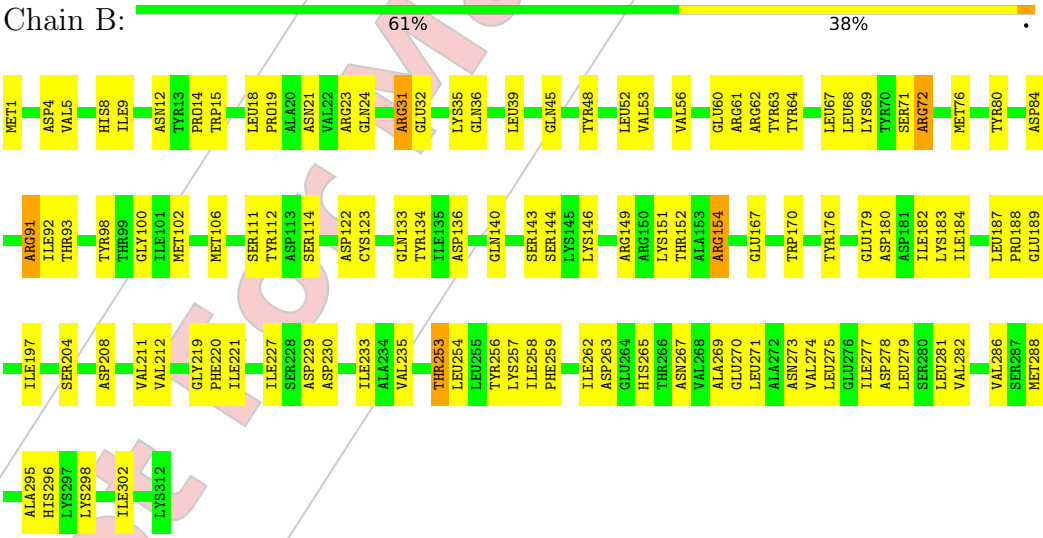
• Molecule 1:

Chain A:



• Molecule 2:

Chain B:



• Molecule 3: ARG-HIS-VAL-SER-SER-SER-ASP-ARG-VAL-GLY-LYS-PRO-TYR-ARG-GLY-VAL-LYS-PRO-VAL-PHE-SER

Chain C:

• Molecule 4: ARG-HIS-VAL-SER-SER-SER-ASP-ARG-VAL-GLY-LYS-PRO-TYR-ARG-GLY-VAL-LYS-PRO-VAL-PHE

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	88.21Å 93.56Å 111.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – (Not available) 69.18 – 2.51	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-(Not available)) 99.9 (69.18-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.86 (at 2.51Å)	Xtriage
Refinement program		Depositor
R, R_{free}	(Not available) , (Not available) 0.253 , 0.276	Depositor DCC
R_{free} test set	1598 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	26.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 56.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	5360	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 63.23 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.9866e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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)

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	0.80	0/2481	0.83	0/3357
2	B	0.88	0/2515	0.81	0/3402
3	C	0.63	0/170	0.91	0/227
4	D	0.69	0/164	0.90	0/219
All	All	0.83	0/5330	0.82	0/7205

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9
2	B	0	7
3	C	0	3
4	D	0	3
All	All	0	22

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	125	ARG	Sidechain
1	A	149	ARG	Sidechain
1	A	150	ARG	Sidechain
1	A	154	ARG	Sidechain
1	A	23	ARG	Sidechain
1	A	49	ARG	Sidechain
1	A	62	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	72	ARG	Sidechain
1	A	91	ARG	Sidechain
2	B	154	ARG	Sidechain
2	B	23	ARG	Sidechain
2	B	31	ARG	Sidechain
2	B	61	ARG	Sidechain
2	B	62	ARG	Sidechain
2	B	72	ARG	Sidechain
2	B	91	ARG	Sidechain
3	C	1	ARG	Sidechain
3	C	14	ARG	Sidechain
3	C	8	ARG	Sidechain
4	D	1	ARG	Sidechain
4	D	14	ARG	Sidechain
4	D	8	ARG	Sidechain

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	2428	0	2431	156	1
2	B	2460	0	2462	103	1
3	C	166	0	172	11	0
4	D	160	0	167	7	0
5	S	146	0	0	1	0
All	All	5360	0	5232	264	1

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 25.

All (264) 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:A:254:LEU:HA	1:A:257:LYS:CE	1.72	1.19
1:A:254:LEU:CA	1:A:257:LYS:HE2	1.76	1.16
1:A:278:ASP:HB3	1:A:281:LEU:HD12	1.19	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:LEU:HA	1:A:257:LYS:HE2	1.10	1.08
1:A:108:SER:OG	1:A:110:LYS:HG2	1.59	1.02
1:A:234:ALA:HA	1:A:264:GLU:HG3	1.43	1.01
1:A:39:LEU:HG	1:A:43:ARG:NH2	1.76	0.98
2:B:182:ILE:HD11	2:B:190:LYS:HG3	1.48	0.95
1:A:187:LEU:HD13	1:A:187:LEU:O	1.67	0.94
2:B:15:TRP:HA	2:B:18:LEU:CD1	1.99	0.91
1:A:187:LEU:CD1	1:A:191:CYS:SG	2.58	0.91
1:A:254:LEU:O	1:A:257:LYS:HG2	1.72	0.88
1:A:187:LEU:HD13	1:A:187:LEU:C	1.96	0.85
1:A:179:GLU:N	1:A:179:GLU:OE1	2.10	0.84
1:A:20:ALA:CA	1:A:23:ARG:HH11	1.91	0.84
1:A:20:ALA:HA	1:A:23:ARG:HH11	1.43	0.84
2:B:296:HIS:ND1	2:B:298:LYS:HE2	1.93	0.83
1:A:187:LEU:HD13	1:A:191:CYS:SG	2.19	0.82
1:A:254:LEU:HA	1:A:257:LYS:HG2	1.62	0.82
1:A:39:LEU:CG	1:A:43:ARG:NH2	2.43	0.81
1:A:254:LEU:HA	1:A:257:LYS:CG	2.10	0.81
1:A:269:ALA:HA	1:A:279:LEU:HD13	1.63	0.80
1:A:254:LEU:CA	1:A:257:LYS:HG2	2.10	0.79
1:A:229:ASP:OD1	1:A:279:LEU:HD21	1.82	0.79
1:A:254:LEU:HA	1:A:257:LYS:CD	2.12	0.78
1:A:271:LEU:O	1:A:275:LEU:HB2	1.84	0.78
1:A:8:HIS:CD2	1:A:22:VAL:HG21	2.19	0.77
1:A:181:ASP:O	1:A:184:ILE:HG22	1.84	0.77
1:A:254:LEU:HG	1:A:257:LYS:HE2	1.67	0.76
4:D:4:SER:O	4:D:7:ASP:HB2	1.85	0.76
1:A:195:LYS:HD2	1:A:199:SER:HB2	1.69	0.74
1:A:265:HIS:O	1:A:265:HIS:CD2	2.40	0.74
1:A:234:ALA:CA	1:A:264:GLU:HG3	2.17	0.74
1:A:254:LEU:CB	1:A:257:LYS:HE2	2.18	0.73
1:A:259:PHE:CZ	1:A:294:PHE:HB3	2.23	0.73
2:B:179:GLU:O	2:B:182:ILE:HG22	1.87	0.73
2:B:190:LYS:NZ	4:D:13:TYR:OH	2.22	0.72
2:B:15:TRP:HA	2:B:18:LEU:HD12	1.71	0.72
2:B:267:ASN:HB3	2:B:270:GLU:HB2	1.72	0.72
2:B:288:MET:SD	2:B:292:LEU:HD12	2.29	0.72
2:B:176:TYR:HE1	4:D:9:VAL:HG23	1.56	0.71
2:B:45:GLN:HA	2:B:67:LEU:HD11	1.72	0.71
1:A:190:LYS:NZ	3:C:13:TYR:CZ	2.58	0.71
2:B:133:GLN:N	2:B:133:GLN:OE1	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:LEU:HD11	1:A:191:CYS:SG	2.30	0.70
2:B:91:ARG:HH11	2:B:176:TYR:HD1	1.38	0.70
1:A:254:LEU:O	1:A:257:LYS:CG	2.40	0.70
1:A:278:ASP:HB3	1:A:281:LEU:CD1	2.12	0.69
1:A:262:ILE:HG23	1:A:271:LEU:HD21	1.73	0.69
2:B:296:HIS:CE1	2:B:298:LYS:HE2	2.28	0.69
1:A:8:HIS:HB3	1:A:18:LEU:HD21	1.74	0.69
1:A:254:LEU:C	1:A:257:LYS:HG2	2.13	0.69
2:B:180:ASP:HA	2:B:183:LYS:HD2	1.73	0.68
2:B:15:TRP:HA	2:B:18:LEU:HD11	1.75	0.68
1:A:39:LEU:CD2	1:A:43:ARG:HH22	2.08	0.66
1:A:254:LEU:CG	1:A:257:LYS:HE2	2.26	0.66
1:A:182:ILE:HD12	1:A:185:CYS:SG	2.36	0.66
1:A:227:ILE:HG21	1:A:286:VAL:HG23	1.79	0.65
2:B:229:ASP:OD1	2:B:279:LEU:HD21	1.97	0.65
1:A:145:LYS:HA	1:A:150:ARG:HG2	1.79	0.64
1:A:187:LEU:CD1	1:A:187:LEU:C	2.65	0.64
1:A:176:TYR:CZ	3:C:18:PRO:HB3	2.32	0.64
2:B:235:VAL:HG13	2:B:259:PHE:CE1	2.31	0.64
1:A:176:TYR:CE1	3:C:18:PRO:HB3	2.33	0.64
1:A:51:ASN:O	1:A:54:LYS:HG2	1.99	0.63
1:A:20:ALA:N	1:A:23:ARG:NH1	2.46	0.63
1:A:225:VAL:HG21	1:A:291:ARG:HB2	1.80	0.63
2:B:281:LEU:HD12	2:B:281:LEU:O	1.99	0.63
1:A:18:LEU:HD22	1:A:22:VAL:HG11	1.81	0.62
1:A:108:SER:OG	1:A:110:LYS:CG	2.40	0.62
1:A:265:HIS:O	1:A:265:HIS:CG	2.53	0.62
1:A:39:LEU:CD2	1:A:43:ARG:NH2	2.63	0.62
1:A:187:LEU:N	1:A:188:PRO:HD2	2.14	0.62
1:A:262:ILE:HD13	1:A:271:LEU:HD21	1.82	0.61
1:A:254:LEU:HG	1:A:257:LYS:CE	2.30	0.61
2:B:182:ILE:CD1	2:B:190:LYS:HG3	2.27	0.61
1:A:197:ILE:HB	3:C:14:ARG:HH21	1.64	0.61
1:A:20:ALA:N	1:A:23:ARG:HH11	1.98	0.61
3:C:13:TYR:CE1	3:C:14:ARG:HG3	2.35	0.61
1:A:7:PHE:HA	1:A:10:ARG:HH21	1.65	0.61
1:A:133:GLN:OE1	1:A:133:GLN:N	2.33	0.60
1:A:230:ASP:HA	1:A:267:ASN:HD21	1.65	0.60
1:A:278:ASP:CB	1:A:281:LEU:HD12	2.13	0.60
2:B:143:SER:HA	2:B:146:LYS:HE2	1.84	0.60
1:A:8:HIS:HD2	1:A:22:VAL:HG21	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:233:ILE:HD13	2:B:286:VAL:CG1	2.32	0.60
2:B:265:HIS:O	2:B:265:HIS:CG	2.54	0.60
1:A:68:LEU:HD12	1:A:86:MET:SD	2.42	0.60
2:B:176:TYR:CE1	4:D:9:VAL:HG23	2.35	0.60
2:B:68:LEU:HD23	2:B:92:ILE:HD12	1.84	0.59
2:B:233:ILE:HD13	2:B:286:VAL:HG13	1.84	0.59
1:A:64:TYR:CD2	1:A:85:ILE:HG21	2.37	0.59
1:A:18:LEU:HD11	1:A:33:TYR:CE1	2.37	0.59
2:B:230:ASP:HA	2:B:267:ASN:HD21	1.66	0.59
2:B:235:VAL:HG21	2:B:262:ILE:HB	1.84	0.59
1:A:1:MET:HE3	1:A:43:ARG:HH12	1.68	0.59
2:B:72:ARG:HH11	2:B:100:GLY:HA3	1.67	0.59
1:A:234:ALA:HB2	1:A:298:LYS:HD2	1.84	0.59
1:A:12:ASN:OD1	1:A:52:LEU:N	2.36	0.59
1:A:18:LEU:HD11	1:A:33:TYR:CZ	2.39	0.58
2:B:167:GLU:O	2:B:204:SER:OG	2.20	0.58
1:A:227:ILE:HG21	1:A:286:VAL:CG2	2.33	0.58
2:B:258:ILE:HG12	2:B:277:ILE:HD13	1.85	0.58
1:A:179:GLU:HA	1:A:182:ILE:HG22	1.86	0.57
2:B:256:TYR:CD1	2:B:257:LYS:HD3	2.39	0.57
2:B:194:ASP:OD1	4:D:13:TYR:OH	2.21	0.57
1:A:262:ILE:HG23	1:A:271:LEU:CD2	2.34	0.57
2:B:235:VAL:CG1	2:B:259:PHE:CE1	2.88	0.57
2:B:254:LEU:HD21	2:B:281:LEU:HD21	1.86	0.57
1:A:1:MET:CE	1:A:43:ARG:HH12	2.18	0.56
1:A:262:ILE:CD1	1:A:271:LEU:HD21	2.36	0.56
2:B:1:MET:HE2	2:B:36:GLN:HA	1.88	0.56
1:A:71:SER:OG	1:A:76:MET:HB2	2.06	0.56
2:B:14:PRO:O	2:B:18:LEU:HG	2.05	0.56
1:A:39:LEU:HG	1:A:43:ARG:HH22	1.64	0.55
2:B:48:TYR:CE2	2:B:60:GLU:HB2	2.42	0.55
2:B:64:TYR:CD2	2:B:85:ILE:HG21	2.42	0.55
2:B:227:ILE:HG13	2:B:286:VAL:HG12	1.90	0.54
1:A:14:PRO:HG2	1:A:17:LYS:HG2	1.88	0.54
1:A:234:ALA:HB1	1:A:264:GLU:HG2	1.89	0.54
1:A:39:LEU:HD21	1:A:43:ARG:NH2	2.23	0.54
2:B:112:TYR:HB2	2:B:134:TYR:CD1	2.43	0.54
1:A:125:ARG:O	1:A:164:ILE:HG22	2.08	0.54
2:B:271:LEU:O	2:B:275:LEU:HB2	2.08	0.54
1:A:64:TYR:CG	1:A:85:ILE:HG21	2.42	0.53
1:A:259:PHE:HZ	1:A:294:PHE:O	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:GLU:HA	1:A:211:VAL:HG13	1.91	0.53
1:A:88:LYS:NZ	5:S:124:HOH:O	2.22	0.53
2:B:35:LYS:O	2:B:39:LEU:HG	2.08	0.53
1:A:230:ASP:HA	1:A:267:ASN:ND2	2.23	0.53
2:B:32:GLU:O	2:B:36:GLN:HG2	2.08	0.53
2:B:5:VAL:O	2:B:9:ILE:HG13	2.09	0.52
2:B:143:SER:O	2:B:146:LYS:HG2	2.08	0.52
1:A:45:GLN:HA	1:A:67:LEU:HD11	1.92	0.52
1:A:20:ALA:O	1:A:24:GLN:HB2	2.09	0.52
2:B:12:ASN:OD1	2:B:52:LEU:N	2.42	0.52
1:A:215:LEU:HB3	1:A:221:ILE:HG12	1.91	0.52
1:A:308:HIS:CE1	1:A:310:SER:OG	2.63	0.52
2:B:68:LEU:CD2	2:B:92:ILE:HD12	2.41	0.51
2:B:149:ARG:HH11	2:B:149:ARG:HG2	1.75	0.51
2:B:189:GLU:HA	2:B:211:VAL:HG13	1.91	0.51
2:B:278:ASP:O	2:B:282:VAL:HG13	2.11	0.51
1:A:88:LYS:HG2	1:A:175:GLY:HA2	1.93	0.51
2:B:21:ASN:O	2:B:24:GLN:HG2	2.11	0.51
1:A:103:GLU:HG3	1:A:157:LEU:HD12	1.91	0.51
2:B:31:ARG:O	2:B:35:LYS:HG3	2.10	0.51
1:A:176:TYR:CZ	3:C:12:PRO:HB3	2.47	0.50
1:A:209:TYR:CD2	1:A:311:TRP:HB3	2.47	0.50
2:B:273:ASN:OD1	2:B:274:VAL:N	2.44	0.50
1:A:178:THR:O	1:A:181:ASP:HB2	2.12	0.50
1:A:8:HIS:CB	1:A:18:LEU:HD21	2.42	0.49
1:A:197:ILE:HD13	3:C:14:ARG:HD3	1.94	0.49
2:B:102:MET:O	2:B:106:MET:HB2	2.12	0.49
1:A:234:ALA:HA	1:A:264:GLU:CG	2.30	0.49
2:B:258:ILE:HG12	2:B:277:ILE:CD1	2.42	0.49
1:A:180:ASP:HA	1:A:183:LYS:HD2	1.93	0.49
2:B:254:LEU:O	2:B:258:ILE:HG13	2.13	0.49
2:B:212:VAL:O	2:B:221:ILE:HD11	2.13	0.49
1:A:233:ILE:HD11	1:A:262:ILE:HG21	1.95	0.48
1:A:254:LEU:O	1:A:258:ILE:N	2.35	0.48
1:A:95:PHE:CE1	1:A:127:LEU:CD2	2.96	0.48
1:A:255:LEU:O	1:A:289:TYR:OH	2.30	0.48
2:B:68:LEU:HD23	2:B:92:ILE:CD1	2.42	0.48
2:B:253:THR:O	2:B:257:LYS:HG2	2.13	0.48
2:B:64:TYR:CG	2:B:85:ILE:HG21	2.49	0.48
1:A:87:VAL:HG22	1:A:93:THR:HA	1.96	0.48
1:A:103:GLU:HG3	1:A:157:LEU:CD1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:LEU:H	1:A:188:PRO:HD2	1.79	0.48
2:B:144:SER:OG	2:B:151:LYS:HD2	2.13	0.48
2:B:182:ILE:HD11	2:B:190:LYS:CG	2.30	0.48
1:A:310:SER:O	1:A:311:TRP:HB2	2.13	0.48
1:A:269:ALA:HA	1:A:279:LEU:CD1	2.41	0.47
1:A:272:ALA:O	1:A:276:GLU:N	2.47	0.47
1:A:182:ILE:O	1:A:185:CYS:HB2	2.13	0.47
2:B:19:PRO:HB2	2:B:21:ASN:OD1	2.14	0.47
2:B:235:VAL:CG2	2:B:262:ILE:CG2	2.92	0.47
1:A:161:PRO:HG2	1:A:217:ASN:HA	1.96	0.47
1:A:196:ILE:HA	1:A:200:GLY:O	2.14	0.47
1:A:253:THR:O	1:A:257:LYS:HG2	2.14	0.47
2:B:256:TYR:HD1	2:B:257:LYS:HD3	1.79	0.47
2:B:229:ASP:HB3	2:B:269:ALA:HB2	1.97	0.47
2:B:180:ASP:O	2:B:184:ILE:HD12	2.15	0.47
1:A:170:TRP:CZ2	1:A:291:ARG:HA	2.50	0.46
2:B:227:ILE:HD13	2:B:227:ILE:HA	1.83	0.46
2:B:84:ASP:O	2:B:88:LYS:HB2	2.15	0.46
2:B:15:TRP:CE3	2:B:18:LEU:HD12	2.51	0.46
2:B:4:ASP:O	2:B:8:HIS:ND1	2.43	0.46
1:A:20:ALA:CA	1:A:23:ARG:NH1	2.69	0.46
1:A:21:ASN:OD1	1:A:22:VAL:N	2.49	0.46
1:A:113:ASP:OD2	1:A:131:ARG:NH2	2.46	0.46
2:B:53:VAL:HG21	2:B:63:TYR:CE2	2.51	0.46
1:A:15:TRP:O	1:A:18:LEU:HB2	2.16	0.45
1:A:258:ILE:O	1:A:262:ILE:HG12	2.17	0.45
1:A:95:PHE:CE1	1:A:127:LEU:HD22	2.51	0.45
2:B:136:ASP:O	2:B:140:GLN:HG3	2.17	0.45
2:B:279:LEU:O	2:B:282:VAL:HG22	2.16	0.45
1:A:167:GLU:HB2	1:A:170:TRP:CD1	2.52	0.45
1:A:193:VAL:HA	1:A:196:ILE:HD12	1.98	0.45
2:B:288:MET:SD	2:B:292:LEU:CD1	3.03	0.45
1:A:181:ASP:HB3	1:A:220:PHE:CZ	2.51	0.45
1:A:257:LYS:O	1:A:260:VAL:HG12	2.17	0.45
2:B:80:TYR:OH	2:B:122:ASP:OD2	2.30	0.45
1:A:235:VAL:O	1:A:264:GLU:OE2	2.35	0.45
1:A:258:ILE:O	1:A:262:ILE:CG1	2.65	0.45
3:C:13:TYR:CD1	3:C:14:ARG:N	2.85	0.45
3:C:16:VAL:O	3:C:16:VAL:HG13	2.16	0.45
1:A:33:TYR:O	1:A:37:VAL:HG23	2.17	0.45
2:B:68:LEU:HD12	2:B:68:LEU:HA	1.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:71:SER:OG	2:B:76:MET:HB2	2.17	0.45
2:B:235:VAL:HG23	2:B:262:ILE:HG22	1.98	0.45
1:A:31:ARG:HA	1:A:31:ARG:HD3	1.82	0.44
2:B:72:ARG:NH1	2:B:100:GLY:HA3	2.32	0.44
2:B:235:VAL:HG23	2:B:262:ILE:CG2	2.48	0.44
1:A:48:TYR:CZ	1:A:54:LYS:HA	2.53	0.44
2:B:270:GLU:O	2:B:273:ASN:OD1	2.36	0.44
1:A:179:GLU:O	1:A:182:ILE:HG22	2.18	0.44
2:B:230:ASP:HA	2:B:267:ASN:ND2	2.32	0.44
2:B:122:ASP:CG	2:B:292:LEU:HD21	2.38	0.44
2:B:219:GLY:HA3	4:D:3:VAL:HG22	1.99	0.44
1:A:18:LEU:O	1:A:23:ARG:NH1	2.51	0.43
2:B:98:TYR:HD1	2:B:123:CYS:HG	1.65	0.43
2:B:235:VAL:HG13	2:B:259:PHE:HE1	1.79	0.43
2:B:1:MET:HE2	2:B:36:GLN:CA	2.48	0.43
1:A:32:GLU:O	1:A:36:GLN:HG3	2.19	0.43
2:B:184:ILE:HG22	2:B:184:ILE:O	2.19	0.43
1:A:5:VAL:HG11	1:A:36:GLN:NE2	2.34	0.43
1:A:7:PHE:CE1	1:A:11:HIS:CD2	3.07	0.43
1:A:39:LEU:CG	1:A:43:ARG:HH22	2.20	0.43
2:B:208:ASP:OD2	2:B:211:VAL:HG23	2.19	0.43
2:B:220:PHE:CD1	2:B:220:PHE:N	2.84	0.43
1:A:182:ILE:HA	1:A:185:CYS:SG	2.59	0.42
2:B:290:CYS:HA	2:B:295:ALA:O	2.19	0.42
1:A:115:LEU:HD23	1:A:115:LEU:HA	1.86	0.42
2:B:302:ILE:HG13	2:B:302:ILE:O	2.18	0.42
1:A:192:ALA:O	1:A:196:ILE:HG13	2.20	0.42
2:B:167:GLU:HB2	2:B:170:TRP:CD1	2.53	0.42
2:B:87:VAL:HG22	2:B:93:THR:HA	2.01	0.42
1:A:84:ASP:O	1:A:88:LYS:HB2	2.19	0.42
1:A:254:LEU:O	1:A:257:LYS:N	2.51	0.42
1:A:39:LEU:CG	1:A:43:ARG:HH21	2.29	0.42
1:A:58:LYS:HA	1:A:58:LYS:HD3	1.78	0.42
1:A:182:ILE:O	1:A:182:ILE:HG13	2.19	0.42
1:A:259:PHE:HD1	1:A:259:PHE:HA	1.73	0.42
2:B:152:THR:HG23	2:B:154:ARG:H	1.85	0.42
1:A:18:LEU:O	1:A:23:ARG:CZ	2.68	0.42
1:A:259:PHE:CZ	1:A:294:PHE:O	2.73	0.42
2:B:179:GLU:HG2	4:D:13:TYR:HA	2.02	0.41
1:A:68:LEU:HD21	1:A:97:TYR:HD1	1.84	0.41
1:A:252:GLU:HB3	1:A:253:THR:H	1.65	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:VAL:O	1:A:286:VAL:HG22	2.21	0.41
1:A:169:TRP:CZ3	1:A:297:LYS:HD2	2.55	0.41
2:B:187:LEU:HB2	2:B:188:PRO:HD3	2.03	0.41
2:B:277:ILE:HG22	2:B:278:ASP:N	2.35	0.41
2:B:193:VAL:O	2:B:197:ILE:HG13	2.21	0.41
1:A:15:TRP:CE2	1:A:30:GLN:HB2	2.56	0.41
3:C:10:GLY:O	3:C:11:LYS:C	2.58	0.41
2:B:45:GLN:HB3	2:B:67:LEU:HD21	2.03	0.40
1:A:177:ILE:HG23	3:C:13:TYR:HB3	2.03	0.40
1:A:271:LEU:O	1:A:275:LEU:N	2.50	0.40
1:A:134:TYR:CE2	1:A:138:MET:HG3	2.56	0.40
2:B:262:ILE:HG12	2:B:271:LEU:HD21	2.04	0.40
1:A:39:LEU:HD11	1:A:43:ARG:HH21	1.87	0.40
1:A:149:ARG:HG2	1:A:149:ARG:NH1	2.35	0.40
2:B:111:SER:O	2:B:114:SER:OG	2.35	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:LYS:O	2:B:69:LYS:NZ[3_645]	1.20	1.00

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	292/296 (99%)	286 (98%)	6 (2%)	0	100	100
2	B	295/299 (99%)	293 (99%)	2 (1%)	0	100	100
3	C	19/21 (90%)	18 (95%)	1 (5%)	0	100	100
4	D	18/20 (90%)	17 (94%)	1 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	624/636 (98%)	614 (98%)	10 (2%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	272/272 (100%)	270 (99%)	2 (1%)	84 84
2	B	275/275 (100%)	272 (99%)	3 (1%)	73 73
3	C	19/19 (100%)	19 (100%)	0	100 100
4	D	18/18 (100%)	17 (94%)	1 (6%)	21 21
All	All	584/584 (100%)	578 (99%)	6 (1%)	76 76

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	160	LYS
1	A	275	LEU
2	B	56	VAL
2	B	253	THR
2	B	263	ASP
4	D	9	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	36	GLN
1	A	265	HIS
1	A	306	GLN
2	B	11	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 monosaccharides 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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	236:PRO	C	250:TYR	N	22.70
1	A	236:PRO	C	252:GLU	N	20.68

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.