Full wwPDB X-ray Structure Validation Report (i)

Nov 15, 2023 – 12:41 AM JST

PDB ID	:	6IOE
Title	:	Crystal structure of the CysR-CTLD2 fragment of human MR at basic pH (pH 8.5)
Authors	:	Hu, Z.; He, Y.
Deposited on	:	2018-10-30
Resolution	:	2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

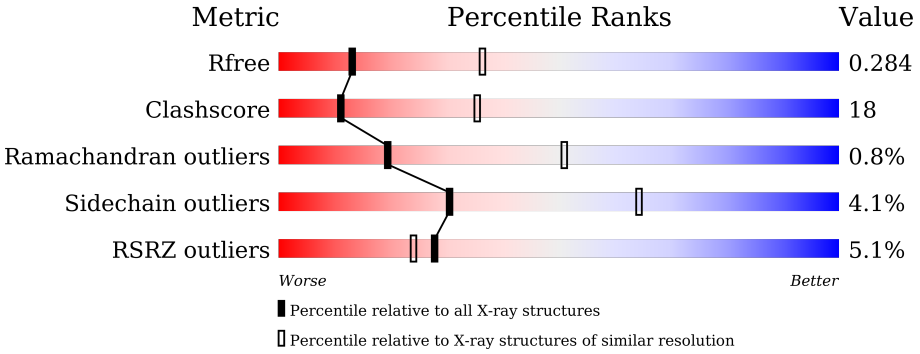
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	475	3% 65% 28% • •
1	B	475	7% 59% 31% • 6%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 7242 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 Macrophage mannose receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	454	3654	2317	618	693	26	0	0	0
1	B	446	3588	2282	603	677	26	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

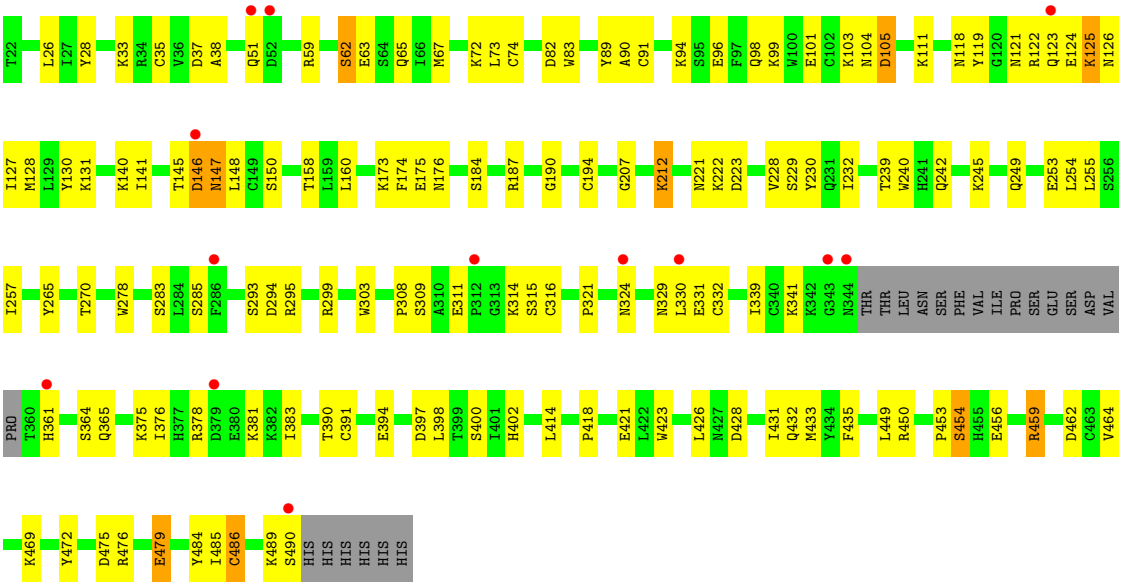
Chain	Residue	Modelled	Actual	Comment	Reference
A	491	HIS	-	expression tag	UNP P22897
A	492	HIS	-	expression tag	UNP P22897
A	493	HIS	-	expression tag	UNP P22897
A	494	HIS	-	expression tag	UNP P22897
A	495	HIS	-	expression tag	UNP P22897
A	496	HIS	-	expression tag	UNP P22897
B	491	HIS	-	expression tag	UNP P22897
B	492	HIS	-	expression tag	UNP P22897
B	493	HIS	-	expression tag	UNP P22897
B	494	HIS	-	expression tag	UNP P22897
B	495	HIS	-	expression tag	UNP P22897
B	496	HIS	-	expression tag	UNP P22897

3 Residue-property plots (i)

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

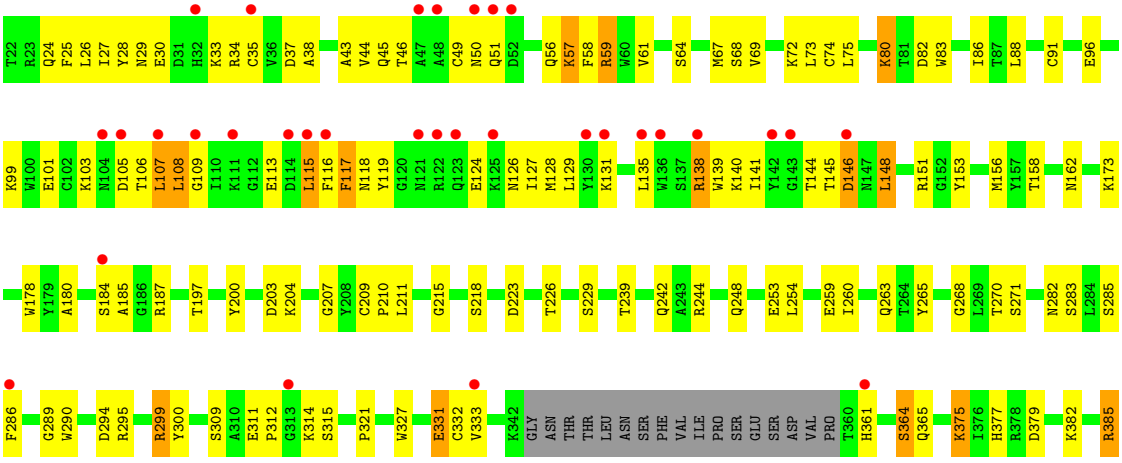
• Molecule 1: Macrophage mannose receptor 1

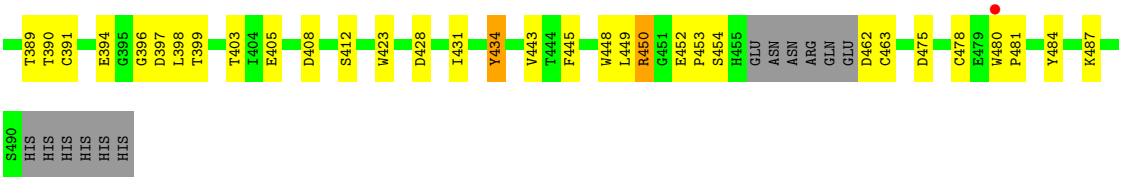
Chain A:



• Molecule 1: Macrophage mannose receptor 1

Chain B:




T389
T390
C391
E394
G395
G396
D397
L398
T399
T403
I404
E405
D408
S412
W423
D428
I431
Y434
V443
T444
F445
W448
L449
R450
G451
E452
P453
S454
H455
GLU
ASN
ASN
ARG
GLN
GLU
D462
C463
D475
C478
E479
W480
P481
Y484
K487
S490
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	241.43Å 72.24Å 109.53Å 90.00° 114.51° 90.00°	Depositor
Resolution (Å)	29.85 – 2.90 29.85 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.0 (29.85-2.90) 97.0 (29.85-2.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 2.90Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.236 , 0.284 0.236 , 0.284	Depositor DCC
R_{free} test set	2006 reflections (5.38%)	wwPDB-VP
Wilson B-factor (Å^2)	55.5	Xtriage
Anisotropy	1.123	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 50.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.025 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7242	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.85% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.34	0/3756	0.60	3/5090 (0.1%)
1	B	0.42	1/3689 (0.0%)	0.73	5/4999 (0.1%)
All	All	0.38	1/7445 (0.0%)	0.67	8/10089 (0.1%)

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	B	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	80	LYS	CE-NZ	6.91	1.66	1.49

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	108	LEU	CB-CG-CD1	-17.17	81.82	111.00
1	B	108	LEU	CB-CG-CD2	11.06	129.80	111.00
1	B	57	LYS	CD-CE-NZ	-7.00	95.60	111.70
1	B	375	LYS	CG-CD-CE	-6.90	91.20	111.90
1	A	331	GLU	CA-CB-CG	-6.50	99.09	113.40
1	A	96	GLU	CA-CB-CG	5.70	125.94	113.40
1	B	50	ASN	C-N-CA	-5.21	108.67	121.70
1	A	479	GLU	C-N-CA	5.04	134.30	121.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	103	LYS	Peptide
1	B	107	LEU	Peptide
1	B	115	LEU	Peptide
1	B	450	ARG	Peptide

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	3654	0	3463	113	1
1	B	3588	0	3406	142	1
All	All	7242	0	6869	253	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 18.

All (253) 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:314:LYS:NZ	1:A:316:CYS:H	1.24	1.36
1:B:289:GLY:HA2	1:B:450:ARG:HB3	1.31	1.10
1:B:26:LEU:HD12	1:B:51:GLN:HG2	1.24	1.09
1:A:140:LYS:NZ	1:A:146:ASP:O	1.90	1.04
1:A:314:LYS:HE2	1:A:330:LEU:C	1.81	1.01
1:A:314:LYS:NZ	1:A:316:CYS:N	2.08	1.00
1:A:140:LYS:NZ	1:A:146:ASP:C	2.19	0.96
1:A:314:LYS:HZ2	1:A:316:CYS:N	1.63	0.95
1:A:314:LYS:NZ	1:A:315:SER:H	1.70	0.90
1:B:450:ARG:HA	1:B:452:GLU:H	1.37	0.89
1:A:314:LYS:HZ1	1:A:316:CYS:H	1.14	0.89
1:A:140:LYS:HZ3	1:A:146:ASP:C	1.74	0.88
1:B:26:LEU:HD12	1:B:51:GLN:CG	2.03	0.88
1:A:314:LYS:HZ2	1:A:316:CYS:H	0.92	0.87
1:A:253:GLU:HG2	1:A:294:ASP:HB3	1.56	0.86
1:B:311:GLU:HB2	1:B:314:LYS:HG2	1.58	0.83
1:A:314:LYS:HE2	1:A:330:LEU:O	1.77	0.83
1:A:221:ASN:ND2	1:A:265:TYR:OH	2.11	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:LEU:CD1	1:B:51:GLN:HG2	2.09	0.81
1:A:314:LYS:HZ3	1:A:315:SER:H	1.30	0.79
1:A:459:ARG:NH1	1:A:462:ASP:OD1	2.18	0.77
1:A:391:CYS:HG	1:A:486:CYS:CB	1.97	0.77
1:B:108:LEU:HD13	1:B:148:LEU:HD11	1.67	0.76
1:A:391:CYS:SG	1:A:486:CYS:HB3	2.25	0.75
1:A:103:LYS:O	1:A:105:ASP:N	2.20	0.74
1:A:239:THR:OG1	1:A:332:CYS:O	2.06	0.73
1:B:59:ARG:NH1	1:B:180:ALA:O	2.22	0.72
1:B:197:THR:HG21	1:B:203:ASP:HB2	1.71	0.72
1:B:45:GLN:HA	1:B:127:ILE:HG12	1.72	0.71
1:A:314:LYS:NZ	1:A:315:SER:N	2.39	0.71
1:A:314:LYS:HZ2	1:A:315:SER:N	1.89	0.70
1:B:283:SER:HB3	1:B:450:ARG:HE	1.56	0.70
1:A:140:LYS:HE2	1:A:145:THR:C	2.13	0.68
1:A:221:ASN:O	1:A:230:TYR:N	2.27	0.67
1:B:399:THR:HA	1:B:487:LYS:HB2	1.76	0.67
1:B:449:LEU:O	1:B:452:GLU:HB2	1.94	0.67
1:B:299:ARG:HG3	1:B:443:VAL:HG11	1.77	0.67
1:A:314:LYS:HE3	1:A:329:ASN:HB2	1.78	0.66
1:A:423:TRP:HB2	1:A:484:TYR:HB3	1.77	0.66
1:B:408:ASP:O	1:B:412:SER:OG	2.13	0.65
1:A:426:LEU:HD23	1:A:464:VAL:HG21	1.78	0.65
1:A:391:CYS:SG	1:A:486:CYS:CB	2.83	0.65
1:B:223:ASP:HB3	1:B:265:TYR:CZ	2.31	0.64
1:A:140:LYS:HZ3	1:A:147:ASN:CA	2.11	0.64
1:B:239:THR:HG23	1:B:242:GLN:H	1.63	0.63
1:A:295:ARG:HG2	1:A:295:ARG:HH11	1.63	0.63
1:B:390:THR:O	1:B:394:GLU:HG3	1.99	0.62
1:B:223:ASP:OD1	1:B:226:THR:OG1	2.14	0.62
1:B:428:ASP:OD1	1:B:462:ASP:HB3	2.00	0.62
1:B:364:SER:O	1:B:365:GLN:HB2	2.00	0.62
1:B:73:LEU:HB2	1:B:88:LEU:HB3	1.82	0.61
1:B:480:TRP:N	1:B:480:TRP:CD1	2.69	0.61
1:B:144:THR:HG22	1:B:145:THR:H	1.66	0.61
1:A:140:LYS:HZ3	1:A:147:ASN:N	1.98	0.60
1:B:428:ASP:HB2	1:B:431:ILE:O	2.01	0.60
1:B:162:ASN:ND2	1:B:204:LYS:O	2.34	0.60
1:B:223:ASP:HB3	1:B:265:TYR:CE1	2.35	0.60
1:B:289:GLY:HA2	1:B:450:ARG:CB	2.20	0.60
1:B:45:GLN:HB3	1:B:126:ASN:HA	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:LEU:HD13	1:B:311:GLU:HG2	1.84	0.59
1:A:239:THR:HG23	1:A:242:GLN:H	1.68	0.59
1:A:82:ASP:OD1	1:A:83:TRP:N	2.36	0.59
1:B:259:GLU:OE2	1:B:299:ARG:NH1	2.35	0.59
1:A:314:LYS:HZ1	1:A:316:CYS:N	1.83	0.58
1:B:268:GLY:O	1:B:271:SER:OG	2.21	0.58
1:A:126:ASN:ND2	1:A:127:ILE:O	2.36	0.58
1:A:140:LYS:HZ1	1:A:146:ASP:C	1.96	0.58
1:B:423:TRP:HB2	1:B:484:TYR:HB3	1.86	0.57
1:A:454:SER:OG	1:A:475:ASP:O	2.21	0.57
1:A:222:LYS:HA	1:A:228:VAL:O	2.04	0.57
1:B:286:PHE:HA	1:B:450:ARG:HH22	1.69	0.57
1:A:418:PRO:HB3	1:A:469:LYS:HA	1.85	0.57
1:B:44:VAL:HG11	1:B:88:LEU:HG	1.86	0.57
1:B:28:TYR:O	1:B:140:LYS:N	2.38	0.56
1:B:67:MET:HA	1:B:74:CYS:HA	1.86	0.56
1:B:140:LYS:HZ3	1:B:141:ILE:H	1.54	0.56
1:B:107:LEU:HD11	1:B:116:PHE:HB3	1.87	0.56
1:A:83:TRP:CD1	1:A:128:MET:HE1	2.41	0.55
1:B:140:LYS:HE2	1:B:146:ASP:C	2.26	0.55
1:B:215:GLY:O	1:B:218:SER:OG	2.19	0.55
1:A:212:LYS:HD2	1:A:212:LYS:N	2.22	0.55
1:A:140:LYS:HE2	1:A:146:ASP:N	2.22	0.55
1:B:253:GLU:HG2	1:B:294:ASP:HB3	1.88	0.55
1:B:244:ARG:O	1:B:248:GLN:HG3	2.07	0.55
1:B:115:LEU:HB2	1:B:129:LEU:HD21	1.89	0.55
1:B:184:SER:C	1:B:187:ARG:HG3	2.27	0.55
1:B:314:LYS:HD2	1:B:331:GLU:HB3	1.89	0.54
1:A:283:SER:O	1:A:450:ARG:NH1	2.36	0.54
1:B:450:ARG:CA	1:B:452:GLU:H	2.15	0.54
1:A:432:GLN:HG2	1:A:433:MET:HE2	1.90	0.54
1:B:331:GLU:CD	1:B:331:GLU:H	2.11	0.53
1:A:270:THR:HB	1:A:321:PRO:HB3	1.91	0.53
1:A:67:MET:SD	1:A:72:LYS:HA	2.48	0.53
1:A:184:SER:O	1:A:184:SER:OG	2.27	0.53
1:A:390:THR:O	1:A:394:GLU:HG3	2.08	0.53
1:B:28:TYR:CE2	1:B:49:CYS:SG	3.02	0.53
1:B:118:ASN:OD1	1:B:119:TYR:N	2.41	0.53
1:B:454:SER:N	1:B:475:ASP:OD1	2.41	0.52
1:A:397:ASP:OD1	1:A:398:LEU:N	2.43	0.52
1:B:209:CYS:HB2	1:B:211:LEU:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:LEU:CD1	1:B:148:LEU:HD11	2.39	0.52
1:B:200:TYR:O	1:B:204:LYS:HD3	2.10	0.52
1:A:383:ILE:HD12	1:A:383:ILE:H	1.75	0.52
1:B:141:ILE:HD11	1:B:148:LEU:HA	1.92	0.52
1:A:67:MET:HA	1:A:74:CYS:HA	1.92	0.52
1:B:117:PHE:HD2	1:B:139:TRP:CZ3	2.28	0.52
1:A:255:LEU:HD21	1:A:257:ILE:HD11	1.92	0.51
1:B:397:ASP:OD1	1:B:398:LEU:N	2.42	0.51
1:A:376:ILE:HG12	1:A:485:ILE:HG12	1.92	0.51
1:B:49:CYS:HA	1:B:56:GLN:HE22	1.76	0.51
1:B:290:TRP:HD1	1:B:453:PRO:HD2	1.75	0.51
1:B:382:LYS:NZ	1:B:484:TYR:OH	2.43	0.51
1:B:289:GLY:HA3	1:B:448:TRP:HB2	1.92	0.51
1:A:73:LEU:HD23	1:A:90:ALA:HA	1.92	0.51
1:A:245:LYS:O	1:A:249:GLN:HG2	2.11	0.51
1:B:101:GLU:N	1:B:109:GLY:O	2.44	0.50
1:B:375:LYS:HD3	1:B:377:HIS:CD2	2.46	0.50
1:A:173:LYS:HD3	1:A:176:ASN:HA	1.94	0.50
1:B:480:TRP:N	1:B:480:TRP:HD1	2.09	0.50
1:A:428:ASP:HB2	1:A:431:ILE:O	2.12	0.50
1:B:140:LYS:HZ3	1:B:141:ILE:N	2.09	0.50
1:B:283:SER:HB3	1:B:450:ARG:NE	2.26	0.50
1:A:26:LEU:HD12	1:A:51:GLN:HG2	1.94	0.49
1:A:253:GLU:HG3	1:A:254:LEU:N	2.27	0.49
1:B:107:LEU:HG	1:B:108:LEU:C	2.33	0.49
1:A:454:SER:N	1:A:475:ASP:OD1	2.44	0.49
1:A:158:THR:HB	1:A:207:GLY:HA3	1.93	0.49
1:B:27:ILE:CD1	1:B:58:PHE:HB2	2.43	0.49
1:B:26:LEU:HD23	1:B:26:LEU:HA	1.54	0.49
1:B:37:ASP:OD2	1:B:38:ALA:N	2.45	0.49
1:B:72:LYS:HD3	1:B:178:TRP:HB2	1.93	0.49
1:B:253:GLU:HG3	1:B:254:LEU:N	2.27	0.48
1:A:314:LYS:HG3	1:A:329:ASN:HB2	1.95	0.48
1:A:376:ILE:HG13	1:A:485:ILE:HG23	1.95	0.48
1:B:239:THR:OG1	1:B:332:CYS:O	2.32	0.48
1:A:140:LYS:HZ3	1:A:147:ASN:HA	1.76	0.48
1:B:124:GLU:HB3	1:B:128:MET:HE1	1.95	0.48
1:A:364:SER:O	1:A:365:GLN:HB2	2.14	0.48
1:B:24:GLN:O	1:B:151:ARG:NH1	2.47	0.48
1:A:285:SER:O	1:A:450:ARG:NH1	2.47	0.48
1:A:309:SER:OG	1:A:311:GLU:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:GLU:O	1:A:126:ASN:N	2.47	0.48
1:A:278:TRP:HH2	1:A:330:LEU:O	1.97	0.48
1:B:28:TYR:N	1:B:139:TRP:HB3	2.28	0.48
1:A:65:GLN:HE21	1:A:99:LYS:NZ	2.12	0.48
1:A:28:TYR:HD1	1:A:35:CYS:SG	2.37	0.47
1:B:184:SER:CA	1:B:187:ARG:HG3	2.44	0.47
1:B:30:GLU:HA	1:B:33:LYS:HD3	1.97	0.47
1:B:107:LEU:HB2	1:B:138:ARG:NH1	2.28	0.47
1:A:454:SER:OG	1:A:475:ASP:OD1	2.31	0.47
1:B:108:LEU:O	1:B:108:LEU:HG	2.14	0.47
1:A:62:SER:OG	1:A:63:GLU:N	2.48	0.47
1:A:449:LEU:HD12	1:A:472:TYR:HB2	1.95	0.47
1:B:67:MET:HG2	1:B:68:SER:N	2.29	0.47
1:B:187:ARG:HA	1:B:187:ARG:NE	2.29	0.47
1:B:28:TYR:HA	1:B:139:TRP:HD1	1.80	0.47
1:B:29:ASN:ND2	1:B:135:LEU:O	2.46	0.47
1:B:46:THR:HG1	1:B:119:TYR:HE1	1.62	0.47
1:A:314:LYS:CE	1:A:330:LEU:N	2.78	0.46
1:B:43:ALA:HA	1:B:126:ASN:HD21	1.80	0.46
1:B:244:ARG:HA	1:B:254:LEU:HG	1.95	0.46
1:B:452:GLU:OE1	1:B:454:SER:OG	2.32	0.46
1:B:283:SER:O	1:B:450:ARG:NH2	2.48	0.46
1:A:83:TRP:CD2	1:A:128:MET:HE2	2.50	0.46
1:B:80:LYS:NZ	1:B:96:GLU:O	2.48	0.46
1:B:58:PHE:CE2	1:B:68:SER:HB2	2.49	0.46
1:A:83:TRP:HZ2	1:A:121:ASN:HB3	1.80	0.46
1:B:58:PHE:CE2	1:B:75:LEU:HD21	2.49	0.46
1:B:259:GLU:OE2	1:B:434:TYR:OH	2.33	0.46
1:B:35:CYS:O	1:B:46:THR:HA	2.16	0.46
1:B:148:LEU:HD23	1:B:148:LEU:H	1.80	0.46
1:A:221:ASN:O	1:A:229:SER:HA	2.16	0.46
1:B:69:VAL:HG23	1:B:180:ALA:HB3	1.97	0.46
1:B:187:ARG:HA	1:B:187:ARG:HE	1.80	0.46
1:B:64:SER:HB3	1:B:99:LYS:HB3	1.98	0.46
1:B:239:THR:OG1	1:B:333:VAL:HA	2.16	0.46
1:B:397:ASP:O	1:B:487:LYS:N	2.49	0.46
1:A:453:PRO:HB2	1:A:456:GLU:OE2	2.16	0.46
1:A:421:GLU:OE2	1:A:476:ARG:NH1	2.49	0.45
1:B:108:LEU:HD13	1:B:148:LEU:CD1	2.43	0.45
1:B:270:THR:HB	1:B:321:PRO:HB3	1.98	0.45
1:B:285:SER:O	1:B:450:ARG:NH1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:ASN:ND2	1:A:119:TYR:O	2.48	0.45
1:B:144:THR:HG22	1:B:145:THR:N	2.30	0.45
1:A:489:LYS:HD2	1:A:490:SER:H	1.81	0.45
1:A:433:MET:CE	1:A:456:GLU:HB3	2.47	0.45
1:B:74:CYS:N	1:B:91:CYS:SG	2.90	0.45
1:B:86:ILE:HG12	1:B:128:MET:HA	1.98	0.45
1:B:107:LEU:HG	1:B:108:LEU:N	2.32	0.45
1:A:37:ASP:OD2	1:A:38:ALA:N	2.50	0.45
1:A:299:ARG:NH2	1:A:435:PHE:O	2.46	0.45
1:B:82:ASP:OD1	1:B:83:TRP:N	2.50	0.45
1:B:185:ALA:O	1:B:187:ARG:HG2	2.17	0.45
1:A:376:ILE:HD12	1:A:414:LEU:HB2	1.99	0.44
1:B:51:GLN:O	1:B:57:LYS:NZ	2.48	0.44
1:A:89:TYR:HB2	1:A:98:GLN:NE2	2.33	0.44
1:A:303:TRP:CE2	1:A:308:PRO:HG3	2.52	0.44
1:B:105:ASP:HB3	1:B:138:ARG:HH12	1.83	0.44
1:B:403:THR:HG22	1:B:405:GLU:H	1.82	0.44
1:A:184:SER:HB2	1:A:190:GLY:HA2	2.00	0.43
1:A:82:ASP:OD1	1:A:130:TYR:HA	2.18	0.43
1:B:67:MET:SD	1:B:72:LYS:HA	2.58	0.43
1:B:463:CYS:N	1:B:478:CYS:SG	2.91	0.43
1:A:232:ILE:HD13	1:A:339:ILE:HG12	2.00	0.43
1:A:83:TRP:CZ2	1:A:121:ASN:HB3	2.54	0.43
1:A:212:LYS:HD2	1:A:212:LYS:H	1.83	0.43
1:B:146:ASP:OD1	1:B:146:ASP:N	2.51	0.43
1:B:158:THR:HB	1:B:207:GLY:HA3	2.00	0.43
1:A:314:LYS:HE3	1:A:316:CYS:O	2.19	0.43
1:A:314:LYS:HE2	1:A:330:LEU:N	2.34	0.43
1:B:106:THR:HG23	1:B:138:ARG:HB3	2.01	0.43
1:B:61:VAL:HG21	1:B:67:MET:HE3	2.00	0.42
1:A:174:PHE:CE1	1:A:175:GLU:HG3	2.54	0.42
1:B:28:TYR:H	1:B:140:LYS:H	1.68	0.42
1:B:260:ILE:HG13	1:B:434:TYR:CE2	2.54	0.42
1:B:30:GLU:O	1:B:33:LYS:HG2	2.19	0.42
1:B:80:LYS:HD2	1:B:113:GLU:OE1	2.19	0.42
1:B:263:GLN:HE22	1:B:327:TRP:HE1	1.67	0.42
1:A:74:CYS:N	1:A:91:CYS:SG	2.92	0.42
1:B:28:TYR:H	1:B:139:TRP:HB3	1.84	0.42
1:A:240:TRP:HD1	1:A:278:TRP:CE3	2.38	0.42
1:A:140:LYS:HA	1:A:140:LYS:HD2	1.55	0.41
1:B:28:TYR:CZ	1:B:33:LYS:HD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:GLN:HE21	1:B:300:TYR:HE1	1.68	0.41
1:B:34:ARG:NH2	1:B:46:THR:O	2.53	0.41
1:B:391:CYS:O	1:B:396:GLY:N	2.51	0.41
1:A:82:ASP:OD2	1:A:131:LYS:HE3	2.20	0.41
1:B:118:ASN:HA	1:B:139:TRP:HH2	1.85	0.41
1:A:228:VAL:HG11	1:A:341:LYS:HE3	2.02	0.41
1:B:209:CYS:CB	1:B:211:LEU:HD12	2.51	0.41
1:A:141:ILE:HG13	1:A:148:LEU:HG	2.03	0.41
1:A:329:ASN:OD1	1:A:329:ASN:N	2.48	0.41
1:B:403:THR:HG22	1:B:405:GLU:N	2.36	0.41
1:B:385:ARG:O	1:B:389:THR:HG23	2.21	0.41
1:A:400:SER:HG	1:A:402:HIS:CE1	2.38	0.41
1:B:80:LYS:CD	1:B:113:GLU:OE1	2.69	0.41
1:B:119:TYR:HE2	1:B:124:GLU:O	2.04	0.41
1:B:282:ASN:HA	1:B:315:SER:O	2.21	0.41
1:B:25:PHE:CE2	1:B:59:ARG:HA	2.56	0.41
1:A:314:LYS:CG	1:A:329:ASN:HB2	2.51	0.40
1:B:144:THR:HG22	1:B:146:ASP:H	1.86	0.40
1:B:156:MET:HG2	1:B:210:PRO:HD2	2.03	0.40
1:A:253:GLU:OE1	1:A:293:SER:OG	2.24	0.40
1:B:185:ALA:C	1:B:187:ARG:HG2	2.42	0.40
1:B:450:ARG:HH11	1:B:450:ARG:HG2	1.85	0.40
1:A:121:ASN:ND2	1:A:123:GLN:HB2	2.37	0.40
1:A:187:ARG:NH2	1:B:312:PRO:HG2	2.37	0.40
1:A:26:LEU:HD23	1:A:26:LEU:HA	1.70	0.40
1:A:101:GLU:OE2	1:A:111:LYS:HG3	2.20	0.40
1:A:122:ARG:HH11	1:A:125:LYS:NZ	2.20	0.40
1:A:147:ASN:O	1:A:150:SER:N	2.51	0.40
1:A:140:LYS:HD2	1:A:141:ILE:H	1.87	0.40
1:B:173:LYS:HB2	1:B:178:TRP:CZ3	2.57	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:479:GLU:OE2	1:B:375:LYS:NZ[1_545]	2.19	0.01

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	450/475 (95%)	411 (91%)	33 (7%)	6 (1%)	12 37
1	B	440/475 (93%)	401 (91%)	38 (9%)	1 (0%)	47 78
All	All	890/950 (94%)	812 (91%)	71 (8%)	7 (1%)	19 51

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	104	ASN
1	A	105	ASP
1	A	125	LYS
1	A	454	SER
1	B	153	TYR
1	A	361	HIS
1	A	147	ASN

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	397/418 (95%)	383 (96%)	14 (4%)	36 70
1	B	390/418 (93%)	372 (95%)	18 (5%)	27 60
All	All	787/836 (94%)	755 (96%)	32 (4%)	30 64

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LYS
1	A	59	ARG
1	A	62	SER
1	A	94	LYS
1	A	146	ASP
1	A	194	CYS
1	A	212	LYS
1	A	223	ASP
1	A	324	ASN
1	A	375	LYS
1	A	378	ARG
1	A	381	LYS
1	A	459	ARG
1	A	486	CYS
1	B	59	ARG
1	B	117	PHE
1	B	131	LYS
1	B	138	ARG
1	B	146	ASP
1	B	148	LEU
1	B	229	SER
1	B	295	ARG
1	B	299	ARG
1	B	309	SER
1	B	331	GLU
1	B	361	HIS
1	B	364	SER
1	B	379	ASP
1	B	385	ARG
1	B	434	TYR
1	B	445	PHE
1	B	481	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	123	GLN
1	A	221	ASN
1	A	344	ASN
1	B	56	GLN
1	B	121	ASN
1	B	126	ASN

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Mol	Chain	Res	Type
1	B	263	GLN
1	B	287	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	454/475 (95%)	0.15	13 (2%)	51	47	38, 59, 87, 128	0
1	B	446/475 (93%)	0.42	33 (7%)	14	11	36, 65, 125, 147	0
All	All	900/950 (94%)	0.29	46 (5%)	28	24	36, 62, 108, 147	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	135	LEU	6.2
1	B	121	ASN	5.7
1	B	47	ALA	4.9
1	B	130	TYR	4.5
1	B	143	GLY	4.3
1	A	146	ASP	4.3
1	B	146	ASP	4.3
1	A	286	PHE	4.2
1	B	48	ALA	4.1
1	A	379	ASP	4.0
1	B	115	LEU	3.8
1	A	123	GLN	3.7
1	B	136	TRP	3.5
1	B	142	TYR	3.4
1	B	122	ARG	3.3
1	B	52	ASP	3.1
1	A	312	PRO	3.1
1	B	480	TRP	3.0
1	B	116	PHE	2.9
1	B	104	ASN	2.9
1	B	107	LEU	2.8
1	A	490	SER	2.8
1	B	125	LYS	2.8
1	A	324	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	361	HIS	2.7
1	A	330	LEU	2.7
1	B	184	SER	2.7
1	A	52	ASP	2.6
1	A	344	ASN	2.6
1	A	361	HIS	2.6
1	B	109	GLY	2.6
1	B	111	LYS	2.5
1	B	32	HIS	2.5
1	B	313	GLY	2.3
1	A	51	GLN	2.3
1	B	50	ASN	2.3
1	B	131	LYS	2.2
1	B	114	ASP	2.2
1	B	51	GLN	2.2
1	B	333	VAL	2.2
1	B	286	PHE	2.1
1	A	343	GLY	2.1
1	B	138	ARG	2.1
1	B	35	CYS	2.1
1	B	123	GLN	2.1
1	B	105	ASP	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.