



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:26 PM GMT

PDB ID : 4ICR
Title : Structural basis for substrate recognition and reaction mechanism of bacterial aminopeptidase peps
Authors : Lee, S.; Kim, K.K.; Ta, M.H.
Deposited on : 2012-12-11
Resolution : 2.17 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

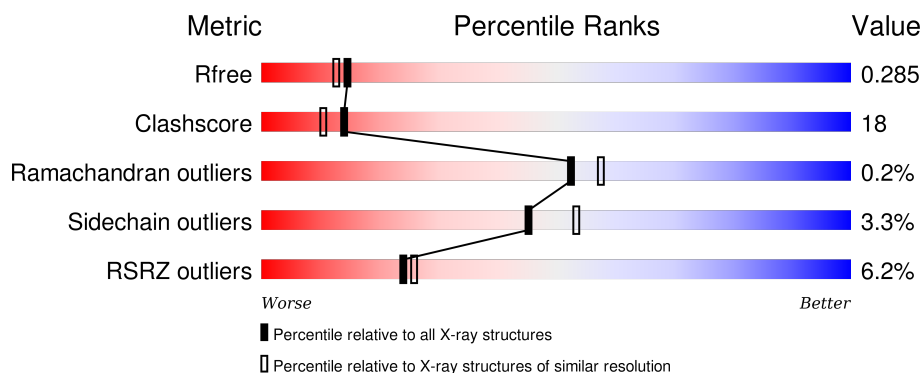
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.17 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	5130 (2.20-2.16)
Clashscore	102246	5965 (2.20-2.16)
Ramachandran outliers	100387	5863 (2.20-2.16)
Sidechain outliers	100360	5864 (2.20-2.16)
RSRZ outliers	91569	5142 (2.20-2.16)

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 $\leq 5\%$. 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	413	<div> <div></div> <div>73% 23% ..</div> </div>
1	B	413	<div> <div>11%</div> <div>70% 24% ..</div> </div>

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	CAC	A	503	-	-	-	X
3	CAC	A	504	-	-	-	X
3	CAC	B	504	-	-	X	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6743 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 Aminopeptidase PepS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	406	Total	C	N	O	S	0	0	0
			3131	1974	532	612	13			
1	B	406	Total	C	N	O	S	0	0	0
			3131	1974	532	612	13			

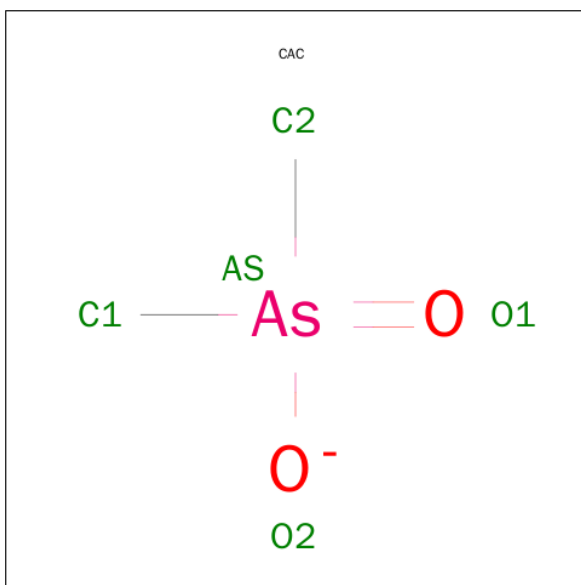
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	343	ASP	GLU	ENGINEERED MUTATION	UNP Q97SP8
B	343	ASP	GLU	ENGINEERED MUTATION	UNP Q97SP8

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is CACODYLATE ION (three-letter code: CAC) (formula: C₂H₆AsO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	As	C	O	0	0
			5	1	2	2		
3	A	1	Total	As	C	O	0	0
			5	1	2	2		
3	B	1	Total	As	C	O	0	0
			5	1	2	2		
3	B	1	Total	As	C	O	0	0
			5	1	2	2		

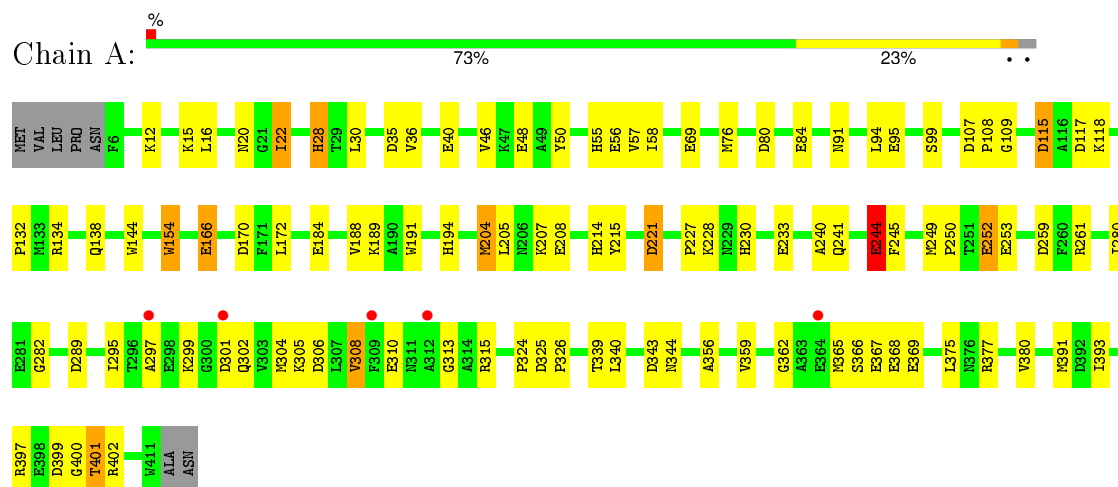
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	228	Total	O	0	0
			228	228		
4	B	229	Total	O	0	0
			229	229		

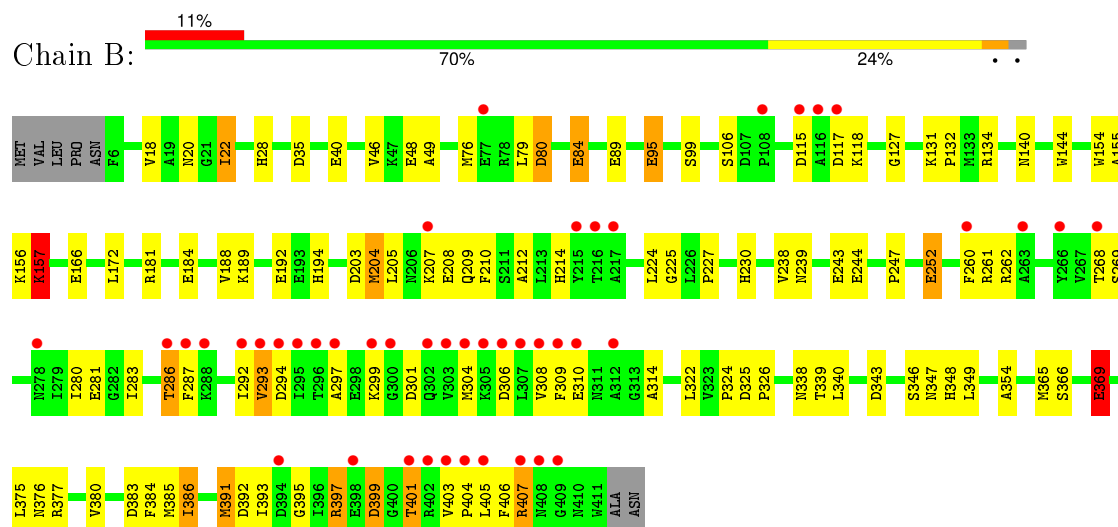
3 Residue-property plots

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: Aminopeptidase PepS



• Molecule 1: Aminopeptidase PepS



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	94.28 Å 185.28 Å 59.24 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.32 – 2.17 46.32 – 2.17	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.32-2.17) 99.5 (46.32-2.17)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.66 (at 2.16 Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.229 , 0.300 0.222 , 0.285	Depositor DCC
R_{free} test set	2818 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	34.5	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 66.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 55646 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6743	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CAC, ZN

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	1.29	15/3195 (0.5%)	0.97	10/4336 (0.2%)
1	B	1.23	15/3195 (0.5%)	0.94	7/4336 (0.2%)
All	All	1.26	30/6390 (0.5%)	0.95	17/8672 (0.2%)

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	244	GLU	CB-CG	21.36	1.92	1.52
1	A	252	GLU	CB-CG	19.34	1.88	1.52
1	A	252	GLU	CD-OE2	18.36	1.45	1.25
1	B	252	GLU	CD-OE2	16.93	1.44	1.25
1	B	252	GLU	CB-CG	15.44	1.81	1.52
1	B	369	GLU	CB-CG	14.54	1.79	1.52
1	B	369	GLU	CD-OE2	12.36	1.39	1.25
1	A	166	GLU	CD-OE2	11.98	1.38	1.25
1	A	166	GLU	CB-CG	11.75	1.74	1.52
1	A	244	GLU	CD-OE2	10.79	1.37	1.25
1	B	166	GLU	CG-CD	9.37	1.66	1.51
1	A	166	GLU	CG-CD	8.35	1.64	1.51
1	B	40	GLU	CG-CD	8.01	1.64	1.51
1	A	252	GLU	CD-OE1	6.76	1.33	1.25
1	A	69	GLU	CD-OE1	-6.64	1.18	1.25
1	B	95	GLU	CG-CD	6.56	1.61	1.51
1	B	243	GLU	CB-CG	6.48	1.64	1.52
1	A	244	GLU	CG-CD	6.47	1.61	1.51
1	A	36	VAL	CB-CG2	6.27	1.66	1.52
1	B	46	VAL	CB-CG2	6.27	1.66	1.52
1	A	154	TRP	CE3-CZ3	5.95	1.48	1.38
1	A	245	PHE	CE2-CZ	5.88	1.48	1.37
1	B	84	GLU	CG-CD	5.80	1.60	1.51
1	A	50	TYR	CD2-CE2	5.77	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	166	GLU	CD-OE1	5.60	1.31	1.25
1	B	49	ALA	CA-CB	5.53	1.64	1.52
1	B	157	LYS	CE-NZ	5.36	1.62	1.49
1	A	40	GLU	CG-CD	5.23	1.59	1.51
1	B	166	GLU	CB-CG	5.11	1.61	1.52
1	B	369	GLU	CG-CD	5.02	1.59	1.51

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	252	GLU	CG-CD-OE1	-11.20	95.90	118.30
1	B	252	GLU	CG-CD-OE1	-10.97	96.36	118.30
1	A	221	ASP	CB-CG-OD1	9.61	126.95	118.30
1	A	244	GLU	CG-CD-OE2	8.74	135.78	118.30
1	B	252	GLU	CG-CD-OE2	8.60	135.50	118.30
1	A	221	ASP	CB-CG-OD2	-7.91	111.18	118.30
1	A	244	GLU	CG-CD-OE1	-7.76	102.79	118.30
1	B	369	GLU	CA-CB-CG	7.59	130.11	113.40
1	A	252	GLU	CG-CD-OE2	7.48	133.25	118.30
1	B	369	GLU	CG-CD-OE1	-6.68	104.95	118.30
1	A	252	GLU	OE1-CD-OE2	6.27	130.83	123.30
1	A	252	GLU	N-CA-CB	6.26	121.86	110.60
1	B	369	GLU	CG-CD-OE2	6.15	130.60	118.30
1	B	407	ARG	NE-CZ-NH1	-5.75	117.42	120.30
1	A	115	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	A	115	ASP	CB-CG-OD1	5.21	122.99	118.30
1	B	80	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3131	0	3052	98	4
1	B	3131	0	3052	129	2

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	10	0	0	1	0
3	B	10	0	0	11	0
4	A	228	0	0	22	1
4	B	229	0	0	16	0
All	All	6743	0	6104	227	4

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 (227) 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:166:GLU:CB	1:A:166:GLU:CG	1.74	1.64
1:B:369:GLU:CB	1:B:369:GLU:CG	1.79	1.59
1:B:252:GLU:CB	1:B:252:GLU:CG	1.81	1.57
1:A:252:GLU:CB	1:A:252:GLU:CG	1.88	1.50
1:A:244:GLU:CB	1:A:244:GLU:CG	1.92	1.45
1:A:194:HIS:HE1	1:A:252:GLU:OE2	1.10	1.27
1:B:194:HIS:HE1	1:B:252:GLU:OE2	1.25	1.19
1:A:194:HIS:CE1	1:A:252:GLU:OE2	2.00	1.14
1:B:118:LYS:HD2	4:B:640:HOH:O	1.49	1.11
1:B:343:ASP:OD2	3:B:504:CAC:AS	2.29	1.10
1:A:115:ASP:OD1	4:A:601:HOH:O	1.69	1.08
1:B:194:HIS:CE1	1:B:252:GLU:OE2	2.06	1.08
1:B:343:ASP:CG	3:B:504:CAC:O1	1.92	1.07
1:A:117:ASP:OD2	4:A:618:HOH:O	1.74	1.05
1:B:118:LYS:CE	4:B:640:HOH:O	2.03	1.04
1:B:397:ARG:HB2	1:B:401:THR:HG23	1.39	1.04
1:B:118:LYS:CD	4:B:640:HOH:O	2.04	1.02
1:B:399:ASP:OD1	1:B:401:THR:HG22	1.57	1.02
1:B:35:ASP:HB2	4:B:613:HOH:O	1.58	1.01
1:B:383:ASP:OD2	3:B:504:CAC:AS	2.38	1.01
1:A:204:MET:HE2	1:A:205:LEU:HA	1.47	0.97
1:A:215:TYR:HD1	1:A:391:MET:HE3	1.29	0.96
1:B:343:ASP:OD2	3:B:504:CAC:O1	1.84	0.95
1:A:367:GLU:OE1	1:A:377:ARG:HD3	1.69	0.92
1:A:204:MET:HE2	1:A:205:LEU:CA	2.00	0.92
1:B:280:ILE:HD13	1:B:304:MET:CE	2.00	0.91
1:B:366:SER:H	1:B:369:GLU:CG	1.85	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ASP:OD1	1:A:108:PRO:HD2	1.74	0.88
1:A:228:LYS:O	4:A:686:HOH:O	1.91	0.87
1:B:280:ILE:HD13	1:B:304:MET:HE3	1.55	0.87
1:A:204:MET:CE	1:A:205:LEU:HA	2.05	0.86
1:A:215:TYR:CD1	1:A:391:MET:HE3	2.11	0.85
1:A:391:MET:HE2	1:A:393:ILE:HD11	1.61	0.83
1:B:157:LYS:HE3	4:B:603:HOH:O	1.78	0.83
1:B:35:ASP:OD2	4:B:755:HOH:O	1.97	0.82
1:B:95:GLU:HG3	4:B:661:HOH:O	1.79	0.82
1:B:268:THR:O	4:B:757:HOH:O	1.96	0.82
1:B:118:LYS:HE3	4:B:640:HOH:O	1.75	0.81
1:B:203:ASP:O	1:B:207:LYS:HG2	1.81	0.81
1:B:399:ASP:OD1	1:B:401:THR:CG2	2.29	0.80
1:B:366:SER:H	1:B:369:GLU:HG3	1.47	0.79
1:B:397:ARG:CB	1:B:401:THR:HG23	2.13	0.79
1:A:204:MET:HE3	1:A:204:MET:O	1.83	0.78
1:A:35:ASP:OD2	4:A:684:HOH:O	2.01	0.78
1:A:400:GLY:O	1:A:402:ARG:NH1	2.19	0.75
1:B:115:ASP:OD2	1:B:117:ASP:HB2	1.87	0.75
1:B:403:VAL:CG1	1:B:404:PRO:HD2	2.17	0.75
1:B:383:ASP:OD2	3:B:504:CAC:O1	2.07	0.73
1:B:366:SER:H	1:B:369:GLU:HG2	1.52	0.73
1:A:107:ASP:OD1	1:A:108:PRO:CD	2.38	0.72
1:A:365:MET:HG2	1:A:369:GLU:HG2	1.69	0.72
1:B:339:THR:CG2	3:B:504:CAC:C1	2.69	0.71
1:B:115:ASP:OD1	1:B:117:ASP:OD2	2.07	0.70
1:B:343:ASP:OD1	3:B:504:CAC:O1	2.09	0.70
1:B:156:LYS:NZ	4:B:683:HOH:O	2.24	0.69
1:B:306:ASP:O	1:B:310:GLU:HB2	1.91	0.69
1:B:339:THR:HG22	3:B:504:CAC:C1	2.23	0.69
1:B:366:SER:OG	1:B:369:GLU:HG2	1.91	0.69
1:A:20:ASN:HD21	1:A:188:VAL:HA	1.59	0.68
1:A:194:HIS:CE1	1:A:252:GLU:CD	2.67	0.68
1:B:306:ASP:HA	1:B:310:GLU:OE2	1.95	0.67
1:B:343:ASP:OD2	3:B:504:CAC:C1	2.42	0.67
1:B:403:VAL:HG12	1:B:404:PRO:HD2	1.77	0.67
1:B:204:MET:HE1	1:B:205:LEU:HA	1.76	0.66
1:A:304:MET:HA	1:A:304:MET:HE2	1.76	0.66
1:B:308:VAL:HA	1:B:314:ALA:HB1	1.77	0.66
1:A:397:ARG:HB2	1:A:401:THR:HG23	1.77	0.66
1:B:287:PHE:CE1	1:B:292:ILE:HG12	2.31	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:LYS:HB3	1:B:132:PRO:HD3	1.76	0.65
1:A:339:THR:HG23	4:A:708:HOH:O	1.96	0.65
1:A:343:ASP:OD1	3:A:504:CAC:C1	2.39	0.64
1:B:280:ILE:CD1	1:B:304:MET:HE1	2.27	0.64
1:A:301:ASP:OD2	1:A:305:LYS:HE2	1.97	0.63
1:B:280:ILE:CD1	1:B:304:MET:CE	2.76	0.62
1:A:15:LYS:NZ	1:A:48:GLU:OE2	2.32	0.61
1:B:280:ILE:HD13	1:B:304:MET:HE1	1.83	0.61
1:A:56:GLU:OE2	1:A:58:ILE:HD11	2.00	0.61
1:B:204:MET:HE2	1:B:204:MET:O	2.01	0.61
1:B:208:GLU:O	1:B:209:GLN:C	2.39	0.61
1:B:366:SER:N	1:B:369:GLU:HG3	2.15	0.60
1:A:391:MET:CE	1:A:393:ILE:HD11	2.31	0.60
1:A:22:ILE:HD11	1:A:144:TRP:HA	1.83	0.60
1:B:210:PHE:CE2	1:B:405:LEU:HD11	2.37	0.60
1:A:252:GLU:HG2	1:A:324:PRO:HD2	1.84	0.59
1:A:46:VAL:HG22	1:A:57:VAL:HG11	1.84	0.59
1:A:304:MET:CE	1:A:304:MET:HA	2.32	0.59
1:A:230:HIS:HE1	4:A:609:HOH:O	1.83	0.59
1:B:376:ASN:C	1:B:377:ARG:HD2	2.22	0.59
1:A:204:MET:HE2	1:A:205:LEU:N	2.17	0.59
1:B:227:PRO:O	1:B:230:HIS:HD2	1.85	0.59
1:A:22:ILE:HG12	1:A:99:SER:HB3	1.85	0.58
1:A:84:GLU:HG3	4:A:788:HOH:O	2.03	0.58
1:B:403:VAL:HG13	1:B:404:PRO:HD2	1.85	0.58
1:A:227:PRO:O	1:A:230:HIS:HD2	1.87	0.58
1:B:252:GLU:CB	1:B:252:GLU:OE1	2.51	0.57
1:B:131:LYS:HD3	1:B:134:ARG:NH1	2.20	0.57
1:B:79:LEU:CD1	1:B:118:LYS:HE2	2.34	0.57
1:A:365:MET:CG	1:A:369:GLU:HG2	2.35	0.57
1:B:20:ASN:H	1:B:20:ASN:HD22	1.53	0.57
1:A:402:ARG:HG3	4:A:679:HOH:O	2.04	0.56
1:B:225:GLY:HA3	1:B:262:ARG:HB2	1.88	0.56
1:A:204:MET:CE	1:A:204:MET:C	2.73	0.56
1:B:127:GLY:HA2	1:B:134:ARG:NH2	2.20	0.56
1:B:286:THR:OG1	1:B:294:ASP:HB3	2.06	0.56
1:B:89:GLU:OE2	4:B:818:HOH:O	2.17	0.56
1:B:115:ASP:OD1	4:B:736:HOH:O	2.17	0.55
1:A:399:ASP:OD2	1:A:401:THR:CG2	2.54	0.55
1:A:108:PRO:HD2	1:A:109:GLY:H	1.71	0.55
1:B:308:VAL:HA	1:B:314:ALA:CB	2.37	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:LYS:CD	1:B:134:ARG:NH1	2.71	0.54
1:A:28:HIS:HD2	4:A:683:HOH:O	1.90	0.54
1:B:383:ASP:CG	3:B:504:CAC:O1	2.46	0.54
1:B:399:ASP:CG	1:B:401:THR:HG22	2.28	0.54
1:B:347:ASN:HD22	1:B:391:MET:CE	2.21	0.54
1:B:204:MET:HE2	1:B:208:GLU:HG3	1.90	0.54
1:B:204:MET:CE	1:B:208:GLU:HG3	2.38	0.54
1:A:134:ARG:O	1:A:138:GLN:HG3	2.08	0.54
1:A:154:TRP:CE3	1:A:172:LEU:HD21	2.43	0.53
1:A:204:MET:CE	1:A:205:LEU:HD23	2.39	0.53
1:B:347:ASN:ND2	1:B:391:MET:HE3	2.24	0.53
1:A:306:ASP:O	1:A:310:GLU:HB2	2.09	0.53
1:B:194:HIS:CE1	1:B:252:GLU:CD	2.82	0.52
1:A:204:MET:HE3	1:A:204:MET:C	2.28	0.52
1:B:347:ASN:HD22	1:B:391:MET:HE3	1.72	0.52
1:A:259:ASP:OD2	4:A:767:HOH:O	2.19	0.52
1:B:189:LYS:HA	1:B:192:GLU:OE1	2.10	0.52
1:B:76:MET:CE	1:B:80:ASP:HB3	2.39	0.52
1:B:84:GLU:HG3	4:B:635:HOH:O	2.10	0.52
1:A:280:ILE:HG23	1:A:299:LYS:O	2.09	0.52
1:B:297:ALA:O	1:B:301:ASP:HB2	2.10	0.51
1:A:191:TRP:CZ3	1:A:194:HIS:HD2	2.29	0.51
1:A:58:ILE:HD13	4:A:632:HOH:O	2.10	0.51
1:B:131:LYS:HD3	1:B:134:ARG:HH12	1.75	0.51
1:A:240:ALA:HB3	1:A:241:GLN:HE22	1.76	0.51
1:B:281:GLU:HB2	1:B:299:LYS:HD2	1.93	0.51
1:A:308:VAL:HG23	1:A:315:ARG:HG2	1.93	0.51
1:A:35:ASP:OD2	4:A:801:HOH:O	2.19	0.51
1:A:402:ARG:CG	4:A:679:HOH:O	2.58	0.51
1:B:214:HIS:NE2	4:B:688:HOH:O	2.20	0.50
1:B:392:ASP:OD1	1:B:407:ARG:HA	2.11	0.50
1:A:204:MET:CE	1:A:208:GLU:HG3	2.41	0.50
1:A:91:ASN:O	1:A:95:GLU:HG3	2.12	0.50
1:A:241:GLN:HG3	4:A:739:HOH:O	2.11	0.49
1:B:269:SER:HA	1:B:385:MET:O	2.13	0.49
1:A:252:GLU:OE1	1:A:252:GLU:CB	2.61	0.49
1:B:325:ASP:HB3	1:B:326:PRO:HD3	1.95	0.49
1:A:22:ILE:HG21	1:A:30:LEU:HD13	1.95	0.48
1:A:204:MET:HE2	1:A:205:LEU:CG	2.43	0.48
1:A:325:ASP:N	1:A:326:PRO:CD	2.77	0.48
1:A:204:MET:HE1	1:A:205:LEU:HD23	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:GLU:OE1	1:B:252:GLU:HB2	2.13	0.48
1:B:106:SER:O	1:B:154:TRP:HB2	2.14	0.48
1:A:359:VAL:HG13	1:A:375:LEU:HD21	1.96	0.48
1:A:240:ALA:HB3	1:A:241:GLN:NE2	2.29	0.47
1:B:22:ILE:HD11	1:B:144:TRP:HA	1.95	0.47
1:B:365:MET:CA	1:B:369:GLU:HG3	2.44	0.47
1:B:204:MET:CE	1:B:205:LEU:HA	2.41	0.47
1:B:393:ILE:HB	1:B:406:PHE:HB2	1.96	0.47
1:B:140:ASN:O	1:B:239:ASN:HA	2.13	0.47
1:A:22:ILE:CG1	1:A:99:SER:HB3	2.44	0.47
1:A:204:MET:HE1	1:A:208:GLU:HG3	1.97	0.47
1:A:58:ILE:CD1	4:A:632:HOH:O	2.63	0.47
1:B:252:GLU:HG2	1:B:324:PRO:HD2	1.96	0.47
1:A:380:VAL:HG13	4:A:760:HOH:O	2.15	0.46
1:B:20:ASN:HD21	1:B:188:VAL:HG13	1.81	0.46
1:B:205:LEU:HD21	1:B:405:LEU:HD13	1.96	0.46
1:B:20:ASN:N	1:B:20:ASN:HD22	2.13	0.46
1:B:20:ASN:N	1:B:20:ASN:ND2	2.64	0.46
1:B:247:PRO:HD2	4:B:678:HOH:O	2.15	0.46
1:B:286:THR:HB	1:B:293:VAL:HG23	1.97	0.46
1:A:313:GLY:HA2	4:A:634:HOH:O	2.15	0.46
1:B:268:THR:HA	1:B:283:ILE:O	2.15	0.46
1:A:227:PRO:O	1:A:230:HIS:CD2	2.68	0.46
1:B:48:GLU:HG2	4:B:787:HOH:O	2.16	0.46
1:A:366:SER:OG	1:A:369:GLU:HB2	2.16	0.46
1:A:356:ALA:O	1:A:362:GLY:HA3	2.16	0.46
1:B:76:MET:HE1	1:B:80:ASP:HB3	1.97	0.45
1:A:253:GLU:H	1:A:344:ASN:ND2	2.14	0.45
1:A:16:LEU:HD12	1:A:20:ASN:ND2	2.30	0.45
1:B:181:ARG:O	1:B:184:GLU:HG3	2.17	0.45
1:B:260:PHE:HB3	1:B:376:ASN:HB2	1.98	0.45
1:B:18:VAL:HA	1:B:22:ILE:HG22	1.98	0.45
1:B:365:MET:HA	1:B:369:GLU:HG3	1.98	0.45
1:B:343:ASP:CG	3:B:504:CAC:AS	3.01	0.45
1:A:108:PRO:CD	1:A:109:GLY:H	2.29	0.45
1:A:339:THR:O	1:A:340:LEU:C	2.54	0.44
1:B:227:PRO:O	1:B:230:HIS:CD2	2.69	0.44
1:B:204:MET:HE1	1:B:205:LEU:CA	2.44	0.44
1:B:376:ASN:O	1:B:377:ARG:HD2	2.17	0.44
1:A:204:MET:CE	1:A:205:LEU:CA	2.77	0.44
1:B:238:VAL:HG22	1:B:244:GLU:HG2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:SER:N	1:B:369:GLU:CG	2.66	0.43
1:B:308:VAL:CG2	1:B:309:PHE:N	2.82	0.43
1:B:405:LEU:HA	1:B:405:LEU:HD23	1.84	0.43
1:B:212:ALA:HB1	1:B:224:LEU:O	2.19	0.43
1:A:249:MET:HA	1:A:250:PRO:HA	1.85	0.43
1:A:325:ASP:HB3	1:A:326:PRO:HD3	2.01	0.42
1:B:348:HIS:HB2	1:B:384:PHE:O	2.19	0.42
1:A:208:GLU:CD	4:A:717:HOH:O	2.57	0.42
1:A:20:ASN:ND2	1:A:188:VAL:HA	2.31	0.42
1:B:322:LEU:HA	1:B:347:ASN:OD1	2.20	0.42
1:B:131:LYS:HD2	1:B:134:ARG:NH1	2.35	0.42
1:B:354:ALA:HB3	1:B:375:LEU:HB3	2.01	0.42
1:B:286:THR:HG1	1:B:294:ASP:HB3	1.82	0.42
1:B:155:ALA:HA	1:B:172:LEU:HD22	2.01	0.42
1:A:94:LEU:HD11	1:A:132:PRO:HB2	2.01	0.41
1:B:286:THR:N	1:B:294:ASP:O	2.47	0.41
1:A:189:LYS:HE2	4:A:635:HOH:O	2.19	0.41
1:A:282:GLY:O	1:A:297:ALA:HA	2.21	0.41
1:B:22:ILE:CG1	1:B:99:SER:HB3	2.50	0.41
1:A:76:MET:SD	1:A:118:LYS:HG2	2.60	0.41
1:B:268:THR:HG23	1:B:283:ILE:O	2.21	0.41
1:B:349:LEU:HG	1:B:386:ILE:HD13	2.03	0.41
1:B:22:ILE:HG12	1:B:99:SER:HB3	2.03	0.41
1:A:80:ASP:HB2	4:A:650:HOH:O	2.19	0.41
1:A:295:ILE:HG21	1:A:308:VAL:CG1	2.51	0.41
1:B:338:ASN:OD1	1:B:340:LEU:HB3	2.21	0.41
1:B:395:GLY:N	1:B:403:VAL:O	2.53	0.41
1:B:209:GLN:HE22	1:B:230:HIS:H	1.68	0.41
1:A:399:ASP:N	1:A:399:ASP:OD2	2.53	0.41
1:A:12:LYS:NZ	1:A:184:GLU:O	2.54	0.40
1:A:166:GLU:OE2	1:A:170:ASP:OD2	2.39	0.40
1:B:366:SER:N	1:B:369:GLU:HG2	2.29	0.40
1:B:304:MET:HA	1:B:304:MET:HE2	2.03	0.40
1:A:359:VAL:HG13	1:A:375:LEU:HD11	2.02	0.40
1:A:302:GLN:NE2	4:A:662:HOH:O	2.49	0.40
1:A:233:GLU:CD	4:A:633:HOH:O	2.59	0.40

All (4) 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:166:GLU:OE2	1:A:368:GLU:OE1[1_554]	1.60	0.60
1:A:221:ASP:OD1	1:B:369:GLU:OE2[3_645]	1.60	0.60
1:A:55:HIS:CE1	4:A:601:HOH:O[4_455]	1.87	0.33
1:A:214:HIS:CE1	1:B:369:GLU:OE2[3_645]	2.14	0.06

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	404/413 (98%)	393 (97%)	11 (3%)	0	100	100
1	B	404/413 (98%)	389 (96%)	13 (3%)	2 (0%)	34	33
All	All	808/826 (98%)	782 (97%)	24 (3%)	2 (0%)	52	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	397	ARG
1	B	386	ILE

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	329/335 (98%)	320 (97%)	9 (3%)	52	62
1	B	329/335 (98%)	316 (96%)	13 (4%)	38	44
All	All	658/670 (98%)	636 (97%)	22 (3%)	45	53

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ILE
1	A	28	HIS
1	A	204	MET
1	A	207	LYS
1	A	244	GLU
1	A	261	ARG
1	A	289	ASP
1	A	308	VAL
1	A	401	THR
1	B	22	ILE
1	B	28	HIS
1	B	157	LYS
1	B	204	MET
1	B	261	ARG
1	B	286	THR
1	B	293	VAL
1	B	346	SER
1	B	369	GLU
1	B	380	VAL
1	B	391	MET
1	B	399	ASP
1	B	401	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	28	HIS
1	A	73	HIS
1	A	91	ASN
1	A	112	ASN
1	A	194	HIS
1	A	209	GLN
1	A	230	HIS
1	A	241	GLN
1	A	331	GLN
1	A	344	ASN
1	B	20	ASN
1	B	112	ASN
1	B	138	GLN
1	B	161	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	194	HIS
1	B	209	GLN
1	B	229	ASN
1	B	230	HIS
1	B	291	GLN
1	B	302	GLN
1	B	344	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\# Z > 2$
3	CAC	A	503	2	0,4,4	0.00	-	0,6,6	0.00	-
3	CAC	A	504	-	0,4,4	0.00	-	0,6,6	0.00	-
3	CAC	B	503	2	0,4,4	0.00	-	0,6,6	0.00	-
3	CAC	B	504	-	0,4,4	0.00	-	0,6,6	0.00	-

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
3	CAC	A	503	2	-	0/0/0/0	0/0/0/0
3	CAC	A	504	-	-	0/0/0/0	0/0/0/0
3	CAC	B	503	2	-	0/0/0/0	0/0/0/0
3	CAC	B	504	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	504	CAC	1	0
3	B	504	CAC	11	0

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 ⓘ

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, 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	406/413 (98%)	0.25	5 (1%) 81 81	18, 33, 50, 61	0
1	B	406/413 (98%)	0.56	45 (11%) 7 8	16, 37, 63, 69	0
All	All	812/826 (98%)	0.41	50 (6%) 24 26	16, 35, 57, 69	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	300	GLY	4.7
1	B	303	VAL	4.5
1	B	286	THR	4.1
1	B	299	LYS	4.0
1	B	297	ALA	3.8
1	A	297	ALA	3.8
1	B	215	TYR	3.8
1	B	266	TYR	3.7
1	B	398	GLU	3.7
1	B	302	GLN	3.7
1	B	307	LEU	3.5
1	B	292	ILE	3.4
1	B	288	LYS	3.3
1	B	310	GLU	3.3
1	B	216	THR	3.1
1	B	295	ILE	3.1
1	B	305	LYS	3.1
1	B	115	ASP	3.0
1	B	403	VAL	3.0
1	B	117	ASP	3.0
1	B	306	ASP	2.9
1	B	404	PRO	2.9
1	B	293	VAL	2.8
1	B	294	ASP	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	312	ALA	2.8
1	B	394	ASP	2.8
1	B	408	ASN	2.6
1	B	278	ASN	2.6
1	B	405	LEU	2.5
1	B	217	ALA	2.5
1	B	309	PHE	2.5
1	B	409	GLY	2.5
1	B	296	THR	2.5
1	B	407	ARG	2.4
1	B	312	ALA	2.4
1	B	268	THR	2.3
1	B	260	PHE	2.3
1	B	308	VAL	2.3
1	B	77	GLU	2.2
1	A	364	GLU	2.2
1	A	309	PHE	2.2
1	B	287	PHE	2.2
1	B	263	ALA	2.1
1	B	304	MET	2.1
1	A	301	ASP	2.1
1	B	402	ARG	2.0
1	B	108	PRO	2.0
1	B	116	ALA	2.0
1	B	401	THR	2.0
1	B	207	LYS	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, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	CAC	A	503	5/5	0.99	0.15	2.99	26,28,30,32	0
3	CAC	A	504	5/5	0.95	0.15	2.20	42,45,51,52	0
3	CAC	B	504	5/5	0.96	0.16	2.02	45,49,52,53	0
3	CAC	B	503	5/5	0.99	0.14	0.95	26,31,33,34	0
2	ZN	B	502	1/1	0.99	0.13	-0.58	31,31,31,31	0
2	ZN	A	502	1/1	1.00	0.10	-0.87	30,30,30,30	0
2	ZN	A	501	1/1	1.00	0.10	-0.98	27,27,27,27	0
2	ZN	B	501	1/1	0.99	0.10	-1.49	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.