Full wwPDB X-ray Structure Validation Report (i)

Mar 10, 2024 – 09:34 AM EDT

PDB ID	:	4NJQ
Title	:	Structural and kinetic bases for the metal preference of the M18 aminopeptidase from Pseudomonas aeruginosa
Authors	:	Nguyen, D.D.; Pandian, R.; Kim, D.Y.; Ha, S.C.; Yun, K.H.; Kim, K.S.; Kim, J.H.; Kim, K.K.
Deposited on	:	2013-11-11
Resolution	:	2.70 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 (i)) were used in the production of this report:

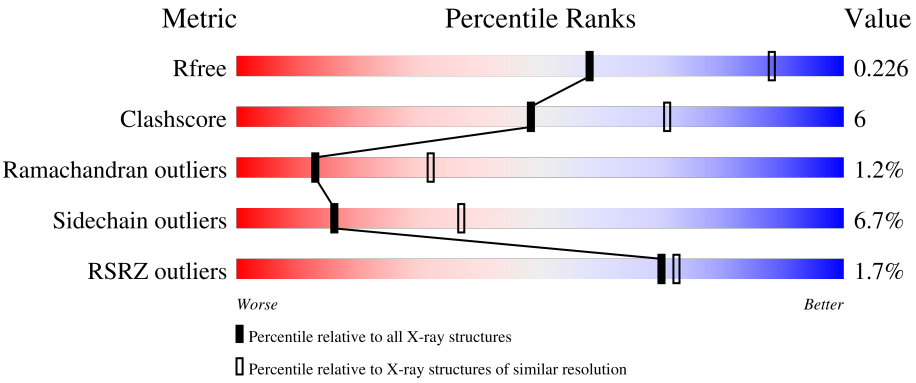
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	429	76% 16% • 5%
1	B	429	3% 81% 14% • •
1	C	429	77% 16% • 5%
1	D	429	78% 15% • 5%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12818 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.

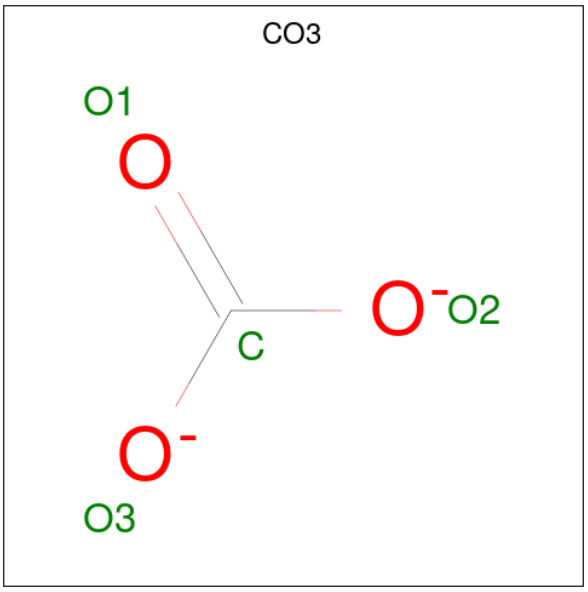
- Molecule 1 is a protein called Probable M18 family aminopeptidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	0	0
			3156	1980	578	590	8			
1	B	410	Total	C	N	O	S	0	0	0
			3174	1990	581	595	8			
1	C	407	Total	C	N	O	S	0	0	0
			3156	1980	578	590	8			
1	D	409	Total	C	N	O	S	0	0	0
			3166	1985	580	593	8			

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

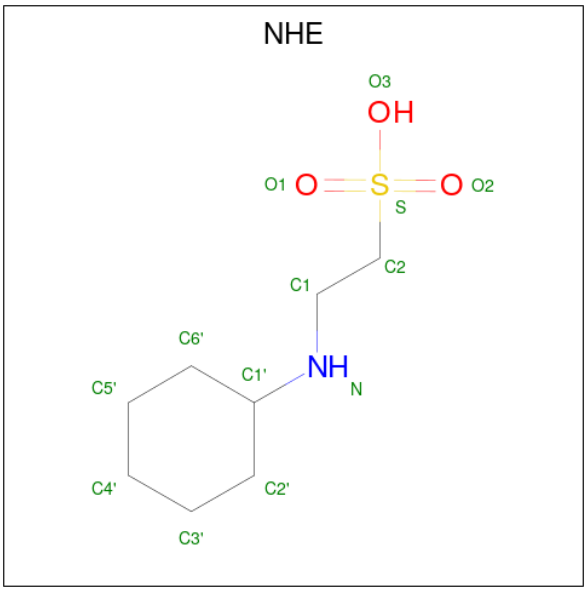
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Co	0	0
			2	2		
2	B	2	Total	Co	0	0
			2	2		
2	C	2	Total	Co	0	0
			2	2		
2	D	2	Total	Co	0	0
			2	2		

- Molecule 3 is CARBONATE ION (three-letter code: CO3) (formula: CO_3).



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

- Molecule 4 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (three-letter code: NHE) (formula: $C_8H_{17}NO_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
4	C	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
4	D	1	Total	C	N	O	S	0	0
			13	8	1	3	1		

- Molecule 5 is water.

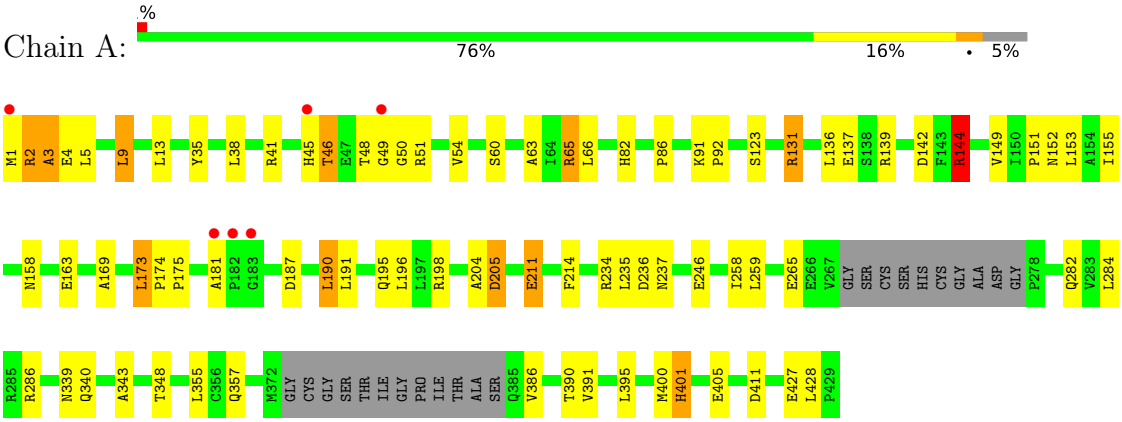
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	27	Total	O	0	0
			27	27		
5	B	22	Total	O	0	0
			22	22		
5	C	24	Total	O	0	0
			24	24		
5	D	30	Total	O	0	0
			30	30		

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.

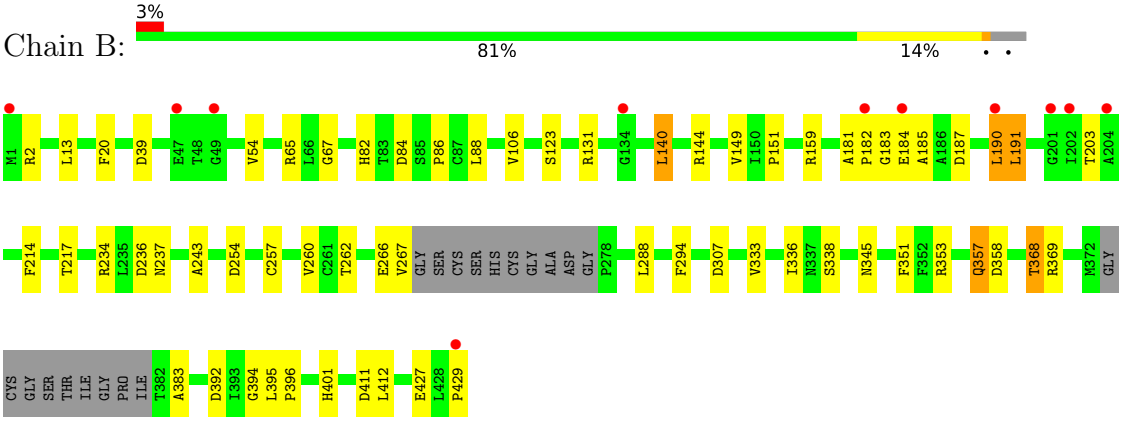
• Molecule 1: Probable M18 family aminopeptidase 2

Chain A:



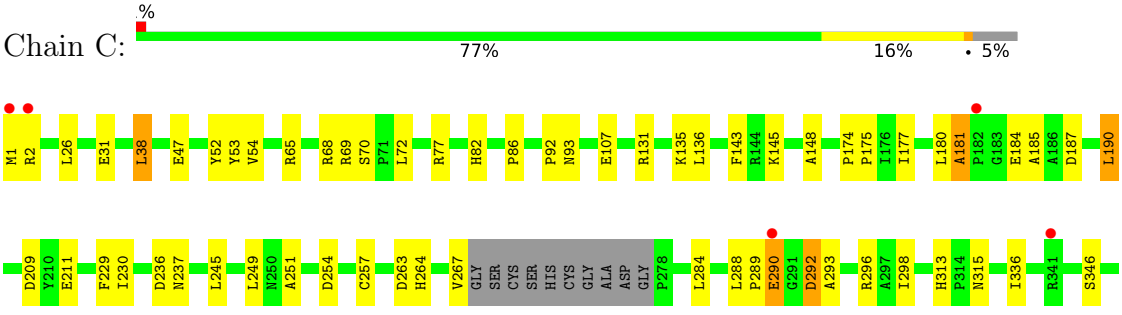
• Molecule 1: Probable M18 family aminopeptidase 2

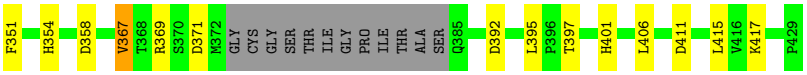
Chain B:



• Molecule 1: Probable M18 family aminopeptidase 2

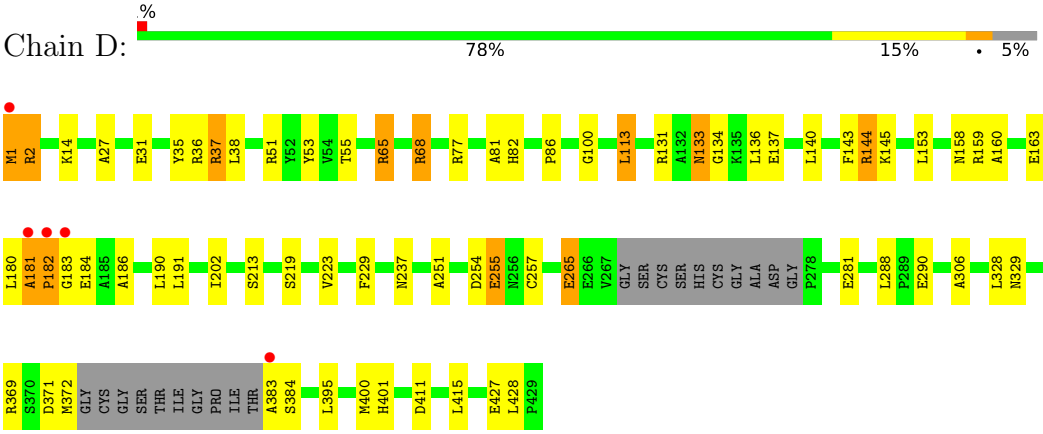
Chain C:





• Molecule 1: Probable M18 family aminopeptidase 2

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	133.21Å 133.21Å 322.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.76 – 2.70 42.98 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.4 (42.76-2.70) 98.5 (42.98-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.58 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.167 , 0.223 0.171 , 0.226	Depositor DCC
R_{free} test set	2920 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	45.2	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 60.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.006 for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k+1/3*l 0.000 for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/3*k+1/3*l 0.009 for -2/3*h-1/3*k-1/3*l,-1/3*h-2/3*k+1/3*l,-4/3*h+4/3*k+1/3*l 0.000 for 1/3*h+2/3*k-1/3*l,-k,-8/3*h-4/3*k-1/3*l 0.005 for -1/3*h-2/3*k+1/3*l,-2/3*h-1/3*k-1/3*l,4/3*h-4/3*k-1/3*l 0.003 for -h,2/3*h+1/3*k+1/3*l,4/3*h+8/3*k-1/3*l 0.025 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12818	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NHE, CO3, CO

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	0.41	0/3221	0.59	1/4372 (0.0%)
1	B	0.42	0/3239	0.56	0/4397
1	C	0.42	0/3221	0.57	0/4372
1	D	0.42	0/3230	0.59	1/4384 (0.0%)
All	All	0.42	0/12911	0.58	2/17525 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2	ARG	C-N-CA	6.09	136.93	121.70
1	D	182	PRO	N-CA-CB	5.56	109.98	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3156	0	3095	56	0
1	B	3174	0	3112	30	0
1	C	3156	0	3095	37	0
1	D	3166	0	3103	37	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
4	A	13	0	17	6	0
4	C	13	0	17	1	0
4	D	13	0	17	3	0
5	A	27	0	0	1	0
5	B	22	0	0	2	0
5	C	24	0	0	1	0
5	D	30	0	0	4	0
All	All	12818	0	12456	151	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 6.

All (151) 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:2:ARG:HB3	1:A:3:ALA:HB3	1.44	0.98
1:B:82:HIS:ND1	5:B:622:HOH:O	2.07	0.86
1:B:84:ASP:OD1	5:B:622:HOH:O	1.96	0.84
1:D:237:ASN:ND2	5:D:630:HOH:O	2.17	0.75
1:A:139:ARG:HH12	4:A:504:NHE:HC22	1.52	0.73
1:A:155:ILE:HB	1:D:113:LEU:HD13	1.72	0.71
4:C:504:NHE:O2	5:C:610:HOH:O	2.09	0.70
1:C:72:LEU:HD11	1:C:293:ALA:HB1	1.76	0.67
1:A:139:ARG:HH12	4:A:504:NHE:C2	2.09	0.66
1:A:2:ARG:CB	1:A:4:GLU:H	2.11	0.64
1:C:284:LEU:HD13	1:C:298:ILE:HD11	1.79	0.64
1:A:187:ASP:HB3	1:A:190:LEU:HB2	1.79	0.64
1:A:86:PRO:HG2	1:A:401:HIS:CG	2.33	0.64
1:A:2:ARG:HB3	1:A:4:GLU:H	1.63	0.63
1:C:292:ASP:OD1	1:C:296:ARG:NH1	2.31	0.63
1:D:100:GLY:HA2	1:D:181:ALA:HB2	1.81	0.63
1:A:41:ARG:HH22	4:A:504:NHE:H5'1	1.63	0.62
1:D:37:ARG:HB2	1:D:53:TYR:CZ	2.35	0.62
1:A:13:LEU:O	1:A:234:ARG:NH2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:ARG:HB2	1:C:257:CYS:HB2	1.82	0.60
1:C:65:ARG:NH1	1:C:251:ALA:HB3	2.17	0.60
1:C:395:LEU:HD22	1:C:411:ASP:HB3	1.82	0.60
1:A:92:PRO:HG3	1:C:336:ILE:HD12	1.84	0.59
1:C:290:GLU:HG3	1:C:292:ASP:HB3	1.85	0.59
1:C:263:ASP:OD1	1:C:264:HIS:N	2.36	0.59
1:D:395:LEU:HD21	1:D:415:LEU:HB2	1.85	0.58
1:A:169:ALA:HA	1:A:173:LEU:HD22	1.87	0.56
1:D:1:MET:HE3	1:D:2:ARG:H	1.70	0.56
1:B:65:ARG:HB3	1:B:257:CYS:HB2	1.87	0.56
1:D:395:LEU:HD22	1:D:411:ASP:HB3	1.87	0.55
1:B:353:ARG:O	1:B:357:GLN:HG2	2.07	0.55
1:D:137:GLU:OE1	4:D:504:NHE:HC11	2.07	0.55
1:B:13:LEU:O	1:B:234:ARG:NH2	2.40	0.54
1:B:86:PRO:HG3	1:B:266:GLU:HG2	1.89	0.53
1:B:82:HIS:CE1	1:B:237:ASN:HB2	2.43	0.53
1:D:65:ARG:NH2	1:D:251:ALA:O	2.30	0.53
1:C:369:ARG:NH2	1:C:371:ASP:OD2	2.38	0.53
1:A:131:ARG:HB3	1:A:131:ARG:HH11	1.74	0.53
1:A:91:LYS:HD3	1:C:367:VAL:HG11	1.91	0.53
1:D:306:ALA:O	5:D:630:HOH:O	2.18	0.53
1:D:65:ARG:HB3	1:D:257:CYS:HB2	1.89	0.52
1:A:51:ARG:HG2	1:A:51:ARG:HH11	1.75	0.52
1:C:26:LEU:HD23	1:C:245:LEU:HD22	1.91	0.52
1:D:153:LEU:HD23	1:D:158:ASN:HB2	1.92	0.52
1:D:68:ARG:NE	1:D:254:ASP:OD1	2.41	0.51
1:B:187:ASP:HB3	1:B:190:LEU:HB2	1.92	0.51
1:D:37:ARG:NH2	5:D:609:HOH:O	2.43	0.51
1:B:20:PHE:HB3	1:B:140:LEU:HD11	1.94	0.50
1:D:77:ARG:HD3	1:D:428:LEU:HD11	1.93	0.50
1:A:51:ARG:NH1	1:A:65:ARG:HG2	2.27	0.49
1:C:229:PHE:HB3	1:C:406:LEU:HD11	1.94	0.49
1:D:143:PHE:O	1:D:145:LYS:N	2.42	0.49
1:A:258:ILE:CD1	1:A:284:LEU:HD21	2.43	0.49
1:C:82:HIS:NE2	1:C:237:ASN:HB2	2.28	0.48
1:A:123:SER:O	1:A:214:PHE:HA	2.12	0.48
1:D:37:ARG:NH1	1:D:38:LEU:O	2.46	0.48
1:A:348:THR:HB	1:A:391:VAL:HB	1.94	0.48
1:C:395:LEU:HD21	1:C:415:LEU:HB2	1.94	0.48
1:D:1:MET:HE3	1:D:2:ARG:N	2.28	0.48
1:A:5:LEU:HD11	1:A:246:GLU:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:ARG:HB3	1:A:3:ALA:CB	2.31	0.48
4:D:504:NHE:H6'1	4:D:504:NHE:HC22	1.96	0.48
1:A:211:GLU:OE1	1:C:346:SER:N	2.47	0.47
1:A:357:GLN:OE1	1:B:131:ARG:NH1	2.42	0.47
1:B:307:ASP:O	1:B:394:GLY:HA3	2.13	0.47
1:B:345:ASN:HB2	1:C:211:GLU:OE2	2.13	0.47
1:A:401:HIS:HA	1:A:405:GLU:OE2	2.13	0.47
1:D:183:GLY:HA3	1:D:184:GLU:HB2	1.97	0.47
1:A:153:LEU:HD23	1:A:158:ASN:HB2	1.96	0.47
1:D:369:ARG:NH1	1:D:371:ASP:OD2	2.48	0.46
1:B:333:VAL:HG23	1:B:396:PRO:HD3	1.97	0.46
1:D:86:PRO:HG2	1:D:401:HIS:CG	2.50	0.46
1:A:2:ARG:CB	1:A:3:ALA:HB3	2.29	0.46
1:A:9:LEU:HD22	1:A:13:LEU:HG	1.98	0.46
1:D:35:TYR:CZ	1:D:51:ARG:HD2	2.51	0.45
1:D:174:PRO:HA	1:D:175:PRO:HD3	1.89	0.45
1:B:368:THR:HG23	1:B:369:ARG:O	2.16	0.45
1:A:149:VAL:O	1:A:151:PRO:HD3	2.16	0.45
1:C:86:PRO:HG2	1:C:401:HIS:CG	2.52	0.45
4:D:504:NHE:H6'1	4:D:504:NHE:C2	2.47	0.45
1:B:86:PRO:HG2	1:B:401:HIS:CG	2.51	0.45
1:D:383:ALA:HA	1:D:384:SER:HA	1.70	0.45
1:A:131:ARG:HD2	1:C:354:HIS:CE1	2.52	0.45
1:A:236:ASP:HA	1:A:237:ASN:HA	1.73	0.45
1:C:38:LEU:HD22	1:C:52:TYR:HB3	1.99	0.45
1:A:137:GLU:OE2	4:A:504:NHE:N	2.50	0.45
1:A:339:ASN:HA	1:B:267:VAL:HG11	1.99	0.45
1:A:282:GLN:O	1:A:286:ARG:HG3	2.16	0.45
1:A:343:ALA:HB3	1:A:390:THR:HB	1.97	0.45
1:A:2:ARG:HB2	1:A:4:GLU:H	1.81	0.44
1:A:131:ARG:NH1	1:A:205:ASP:HB2	2.32	0.44
1:A:136:LEU:HD11	1:C:351:PHE:HA	2.00	0.44
1:B:338:SER:OG	1:C:107:GLU:OE1	2.31	0.44
1:B:236:ASP:HA	1:B:237:ASN:HA	1.78	0.44
1:C:31:GLU:OE2	1:C:53:TYR:OH	2.17	0.44
1:A:400:MET:HA	1:A:401:HIS:HA	1.63	0.44
1:C:181:ALA:N	1:C:184:GLU:OE1	2.42	0.44
1:A:131:ARG:HD2	1:C:354:HIS:ND1	2.33	0.43
1:A:195:GLN:OE1	1:A:198:ARG:NH1	2.44	0.43
1:C:290:GLU:HG2	1:C:293:ALA:H	1.83	0.43
1:D:180:LEU:HD11	1:D:186:ALA:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:400:MET:O	1:D:401:HIS:HB2	2.18	0.43
1:B:288:LEU:HD13	1:B:294:PHE:HA	1.99	0.43
1:C:417:LYS:HE3	1:C:417:LYS:HB2	1.65	0.43
1:D:160:ALA:HB1	1:D:163:GLU:HG3	2.00	0.43
1:B:82:HIS:H	1:B:237:ASN:HD22	1.64	0.43
1:B:243:ALA:HB2	1:B:412:LEU:HD12	2.01	0.43
1:A:63:ALA:HB3	1:A:259:LEU:HB3	2.00	0.43
1:C:369:ARG:HH21	1:C:371:ASP:CG	2.22	0.43
1:B:191:LEU:HD12	1:B:191:LEU:HA	1.86	0.43
1:B:395:LEU:HD22	1:B:411:ASP:HB3	2.01	0.43
1:C:187:ASP:HB3	1:C:190:LEU:HB2	2.01	0.43
1:B:351:PHE:HB2	1:B:429:PRO:HG3	2.01	0.42
1:C:236:ASP:HA	1:C:237:ASN:HA	1.81	0.42
1:D:223:VAL:HG23	1:D:229:PHE:HB2	2.01	0.42
1:A:142:ASP:O	1:A:144:ARG:HG2	2.19	0.42
1:D:27:ALA:O	1:D:31:GLU:HG3	2.20	0.42
1:A:427:GLU:O	1:A:428:LEU:HD23	2.19	0.42
1:D:82:HIS:HB3	1:D:265:GLU:HG3	2.01	0.42
1:D:254:ASP:HB2	1:D:255:GLU:H	1.52	0.42
1:A:234:ARG:NH1	5:A:607:HOH:O	2.41	0.42
1:A:196:LEU:HD23	1:A:196:LEU:HA	1.91	0.41
1:D:14:LYS:HE2	1:D:219:SER:OG	2.19	0.41
1:B:181:ALA:O	1:B:184:GLU:HB2	2.20	0.41
1:C:174:PRO:HA	1:C:175:PRO:HD3	1.88	0.41
1:A:395:LEU:HD22	1:A:411:ASP:HB3	2.01	0.41
1:A:82:HIS:H	1:A:237:ASN:HD22	1.68	0.41
1:A:174:PRO:HA	1:A:175:PRO:HD3	1.89	0.41
1:A:38:LEU:O	1:A:54:VAL:HG23	2.20	0.41
1:A:92:PRO:CG	1:C:336:ILE:HD12	2.50	0.41
1:B:182:PRO:HA	1:B:183:GLY:HA2	1.65	0.41
1:B:123:SER:O	1:B:214:PHE:HA	2.21	0.41
1:B:149:VAL:O	1:B:151:PRO:HD3	2.21	0.41
1:C:298:ILE:HA	1:C:298:ILE:HD13	1.84	0.41
1:A:41:ARG:NH2	4:A:504:NHE:H5'1	2.34	0.41
1:A:131:ARG:HH12	1:A:205:ASP:HB2	1.86	0.41
1:B:67:GLY:HA3	1:B:254:ASP:O	2.21	0.41
1:C:143:PHE:O	1:C:145:LYS:N	2.50	0.41
1:D:81:ALA:HA	5:D:630:HOH:O	2.20	0.41
1:A:82:HIS:NE2	1:A:237:ASN:HB2	2.36	0.41
1:A:35:TYR:CZ	1:A:51:ARG:HD3	2.56	0.40
1:A:49:GLY:HA2	1:A:66:LEU:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:ASN:N	1:D:134:GLY:HA2	2.35	0.40
4:A:504:NHE:H6'2	4:A:504:NHE:HC11	1.33	0.40
1:C:313:HIS:CE1	1:C:315:ASN:HB2	2.56	0.40
1:D:65:ARG:NH2	1:D:251:ALA:HB3	2.37	0.40
1:B:336:ILE:HD13	1:C:92:PRO:HG3	2.03	0.40
1:D:180:LEU:HB3	1:D:181:ALA:H	1.57	0.40
1:D:328:LEU:O	1:D:329:ASN:HB2	2.22	0.40
1:A:49:GLY:N	1:A:50:GLY:HA3	2.36	0.40
1:C:148:ALA:HB2	1:C:177:ILE:HG22	2.03	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	A	401/429 (94%)	377 (94%)	19 (5%)	5 (1%)	13	32
1	B	404/429 (94%)	389 (96%)	12 (3%)	3 (1%)	22	46
1	C	401/429 (94%)	378 (94%)	18 (4%)	5 (1%)	13	32
1	D	403/429 (94%)	380 (94%)	17 (4%)	6 (2%)	10	26
All	All	1609/1716 (94%)	1524 (95%)	66 (4%)	19 (1%)	13	32

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	181	ALA
1	C	289	PRO
1	D	182	PRO
1	A	46	THR
1	A	204	ALA
1	D	133	ASN

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Mol	Chain	Res	Type
1	B	144	ARG
1	B	185	ALA
1	C	185	ALA
1	C	290	GLU
1	D	144	ARG
1	D	255	GLU
1	A	3	ALA
1	A	144	ARG
1	B	383	ALA
1	C	2	ARG
1	D	181	ALA
1	C	181	ALA
1	D	288	LEU

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	330/344 (96%)	308 (93%)	22 (7%)	16	37
1	B	332/344 (96%)	314 (95%)	18 (5%)	22	47
1	C	330/344 (96%)	305 (92%)	25 (8%)	13	30
1	D	330/344 (96%)	306 (93%)	24 (7%)	14	33
All	All	1322/1376 (96%)	1233 (93%)	89 (7%)	16	37

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	9	LEU
1	A	45	HIS
1	A	46	THR
1	A	48	THR
1	A	60	SER
1	A	65	ARG
1	A	131	ARG

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Mol	Chain	Res	Type
1	A	144	ARG
1	A	152	ASN
1	A	163	GLU
1	A	173	LEU
1	A	190	LEU
1	A	191	LEU
1	A	205	ASP
1	A	211	GLU
1	A	235	LEU
1	A	265	GLU
1	A	340	GLN
1	A	355	LEU
1	A	386	VAL
1	A	401	HIS
1	B	2	ARG
1	B	39	ASP
1	B	54	VAL
1	B	88	LEU
1	B	106	VAL
1	B	140	LEU
1	B	159	ARG
1	B	190	LEU
1	B	191	LEU
1	B	203	THR
1	B	217	THR
1	B	260	VAL
1	B	262	THR
1	B	357	GLN
1	B	358	ASP
1	B	368	THR
1	B	392	ASP
1	B	427	GLU
1	C	1	MET
1	C	38	LEU
1	C	47	GLU
1	C	54	VAL
1	C	68	ARG
1	C	69	ARG
1	C	70	SER
1	C	77	ARG
1	C	93	ASN
1	C	131	ARG

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Mol	Chain	Res	Type
1	C	135	LYS
1	C	136	LEU
1	C	180	LEU
1	C	190	LEU
1	C	209	ASP
1	C	230	ILE
1	C	249	LEU
1	C	254	ASP
1	C	267	VAL
1	C	288	LEU
1	C	292	ASP
1	C	358	ASP
1	C	367	VAL
1	C	392	ASP
1	C	397	THR
1	D	1	MET
1	D	2	ARG
1	D	36	ARG
1	D	37	ARG
1	D	55	THR
1	D	65	ARG
1	D	68	ARG
1	D	113	LEU
1	D	131	ARG
1	D	136	LEU
1	D	140	LEU
1	D	144	ARG
1	D	159	ARG
1	D	190	LEU
1	D	191	LEU
1	D	202	ILE
1	D	213	SER
1	D	265	GLU
1	D	281	GLU
1	D	290	GLU
1	D	367	VAL
1	D	368	THR
1	D	372	MET
1	D	427	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	354	HIS

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)

Of 15 ligands modelled in this entry, 8 are monoatomic - leaving 7 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	CO3	B	503	2	2,3,3	0.36	0	2,3,3	0.54	0
3	CO3	C	503	2	2,3,3	0.28	0	2,3,3	0.25	0
4	NHE	C	504	-	13,13,13	1.06	0	16,17,17	3.00	6 (37%)
4	NHE	A	504	-	13,13,13	1.10	1 (7%)	16,17,17	1.87	4 (25%)
4	NHE	D	504	-	13,13,13	1.13	1 (7%)	16,17,17	3.73	7 (43%)
3	CO3	D	503	2	2,3,3	0.33	0	2,3,3	0.39	0
3	CO3	A	503	2	2,3,3	0.30	0	2,3,3	0.35	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NHE	C	504	-	-	5/7/15/15	0/1/1/1
4	NHE	A	504	-	-	2/7/15/15	0/1/1/1
4	NHE	D	504	-	-	2/7/15/15	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	504	NHE	O2-S	2.74	1.53	1.45
4	D	504	NHE	O2-S	2.69	1.53	1.45

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	504	NHE	O1-S-C2	11.54	120.82	106.92
4	C	504	NHE	O2-S-C2	7.24	115.63	106.92
4	D	504	NHE	O2-S-C2	6.08	114.24	106.92
4	C	504	NHE	O1-S-C2	5.76	113.85	106.92
4	A	504	NHE	O1-S-C2	5.18	113.15	106.92
4	D	504	NHE	O2-S-O1	-5.14	96.15	113.95
4	C	504	NHE	O2-S-O1	-4.76	97.49	113.95
4	C	504	NHE	C5'-C6'-C1'	2.89	116.54	111.11
4	A	504	NHE	O3-S-C2	2.86	110.40	105.77
4	C	504	NHE	C2-C1-N	-2.85	103.16	111.25
4	A	504	NHE	O2-S-O1	-2.66	104.75	113.95
4	A	504	NHE	C1-N-C1'	-2.55	109.12	114.14
4	D	504	NHE	C4'-C3'-C2'	2.30	116.11	111.42
4	D	504	NHE	C5'-C6'-C1'	2.18	115.22	111.11
4	D	504	NHE	O3-S-C2	-2.14	102.30	105.77
4	C	504	NHE	C6'-C1'-C2'	-2.11	107.15	110.82
4	D	504	NHE	C6'-C1'-C2'	2.03	114.35	110.82

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	504	NHE	C6'-C1'-N-C1
4	C	504	NHE	C1-C2-S-O2
4	C	504	NHE	C1-C2-S-O3
4	D	504	NHE	C2-C1-N-C1'
4	A	504	NHE	C2-C1-N-C1'
4	C	504	NHE	N-C1-C2-S

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Mol	Chain	Res	Type	Atoms
4	D	504	NHE	N-C1-C2-S
4	C	504	NHE	C1-C2-S-O1
4	C	504	NHE	C2-C1-N-C1'

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	504	NHE	1	0
4	A	504	NHE	6	0
4	D	504	NHE	3	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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	407/429 (94%)	-0.48	6 (1%) 73 76	30, 39, 63, 89	0
1	B	410/429 (95%)	-0.25	11 (2%) 54 55	29, 39, 62, 84	0
1	C	407/429 (94%)	-0.47	5 (1%) 79 80	29, 39, 63, 87	0
1	D	409/429 (95%)	-0.39	6 (1%) 73 76	28, 38, 61, 87	0
All	All	1633/1716 (95%)	-0.40	28 (1%) 70 72	28, 39, 63, 89	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	182	PRO	6.3
1	D	181	ALA	4.3
1	B	182	PRO	3.9
1	A	49	GLY	3.9
1	A	45	HIS	3.8
1	D	383	ALA	3.5
1	C	1	MET	3.5
1	B	49	GLY	3.4
1	B	202	ILE	2.9
1	A	181	ALA	2.9
1	C	182	PRO	2.8
1	B	1	MET	2.7
1	A	182	PRO	2.5
1	A	183	GLY	2.4
1	C	2	ARG	2.4
1	D	341	ARG	2.2
1	B	47	GLU	2.2
1	B	190	LEU	2.2
1	D	1	MET	2.2
1	B	204	ALA	2.1
1	B	184	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	290	GLU	2.1
1	B	201	GLY	2.1
1	B	429	PRO	2.1
1	A	1	MET	2.1
1	B	134	GLY	2.1
1	D	183	GLY	2.0
1	C	341	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NHE	A	504	13/13	0.91	0.18	51,59,72,79	0
4	NHE	D	504	13/13	0.92	0.34	27,40,51,52	0
4	NHE	C	504	13/13	0.93	0.35	11,33,44,45	0
3	CO3	D	503	4/4	0.95	0.13	46,55,55,60	0
3	CO3	C	503	4/4	0.97	0.08	45,46,55,61	0
3	CO3	A	503	4/4	0.98	0.08	44,49,51,54	0
2	CO	D	502	1/1	0.99	0.14	36,36,36,36	0
2	CO	A	501	1/1	0.99	0.12	35,35,35,35	0
3	CO3	B	503	4/4	0.99	0.09	44,45,52,55	0
2	CO	A	502	1/1	0.99	0.10	39,39,39,39	0
2	CO	B	502	1/1	0.99	0.10	40,40,40,40	0
2	CO	C	501	1/1	0.99	0.09	37,37,37,37	0
2	CO	C	502	1/1	0.99	0.08	40,40,40,40	0
2	CO	D	501	1/1	0.99	0.11	38,38,38,38	0
2	CO	B	501	1/1	1.00	0.15	36,36,36,36	0

6.5 Other polymers (i)

There are no such residues in this entry.