



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:27 AM GMT

PDB ID : 2AHR
Title : Crystal Structures of 1-Pyrroline-5-Carboxylate Reductase from Human Pathogen *Streptococcus pyogenes*
Authors : Nocek, B.; Lezondra, L.; Holzle, D.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2005-07-28
Resolution : 2.15 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

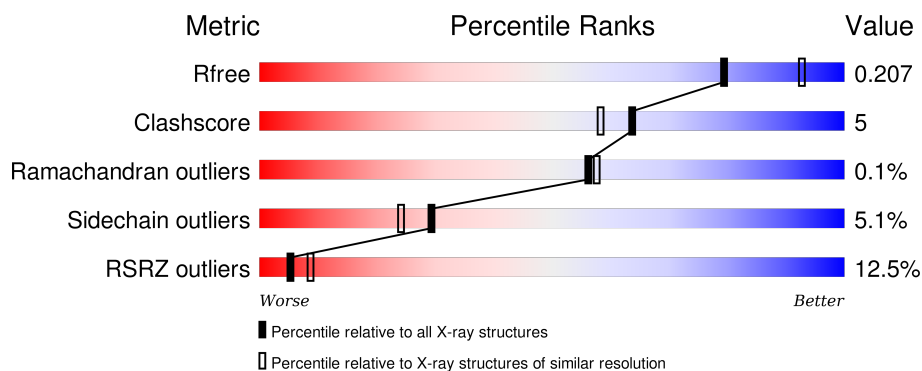
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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	259	<div> <div>9%</div> <div>83%15%</div> </div>
1	B	259	<div> <div>12%</div> <div>92%8%</div> </div>
1	C	259	<div> <div>23%</div> <div>80%16%</div> </div>
1	D	259	<div> <div>3%</div> <div>83%15%</div> </div>
1	E	259	<div> <div>13%</div> <div>88%10%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10547 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 putative pyrroline carboxylate reductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	Se	0	0	0
			1921	1224	319	370	1	7			
1	B	257	Total	C	N	O	S	Se	0	0	0
			1921	1224	319	370	1	7			
1	C	256	Total	C	N	O	S	Se	0	0	0
			1916	1221	318	369	1	7			
1	D	258	Total	C	N	O	S	Se	0	0	0
			1926	1227	320	371	1	7			
1	E	259	Total	C	N	O	S	Se	0	0	0
			1935	1231	322	374	1	7			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	CLONING ARTIFACT	UNP Q9A1S9
A	-1	ASN	-	CLONING ARTIFACT	UNP Q9A1S9
A	0	ALA	-	CLONING ARTIFACT	UNP Q9A1S9
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
A	11	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
A	49	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
A	86	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
A	109	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
A	112	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
A	231	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
B	-2	SER	-	CLONING ARTIFACT	UNP Q9A1S9
B	-1	ASN	-	CLONING ARTIFACT	UNP Q9A1S9
B	0	ALA	-	CLONING ARTIFACT	UNP Q9A1S9
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
B	11	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
B	49	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
B	86	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
B	109	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
B	112	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	231	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
C	-2	SER	-	CLONING ARTIFACT	UNP Q9A1S9
C	-1	ASN	-	CLONING ARTIFACT	UNP Q9A1S9
C	0	ALA	-	CLONING ARTIFACT	UNP Q9A1S9
C	1	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
C	11	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
C	49	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
C	86	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
C	109	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
C	112	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
C	231	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
D	-2	SER	-	CLONING ARTIFACT	UNP Q9A1S9
D	-1	ASN	-	CLONING ARTIFACT	UNP Q9A1S9
D	0	ALA	-	CLONING ARTIFACT	UNP Q9A1S9
D	1	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
D	11	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
D	49	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
D	86	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
D	109	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
D	112	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
D	231	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
E	-2	SER	-	CLONING ARTIFACT	UNP Q9A1S9
E	-1	ASN	-	CLONING ARTIFACT	UNP Q9A1S9
E	0	ALA	-	CLONING ARTIFACT	UNP Q9A1S9
E	1	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
E	11	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
E	49	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
E	86	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
E	109	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
E	112	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
E	231	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

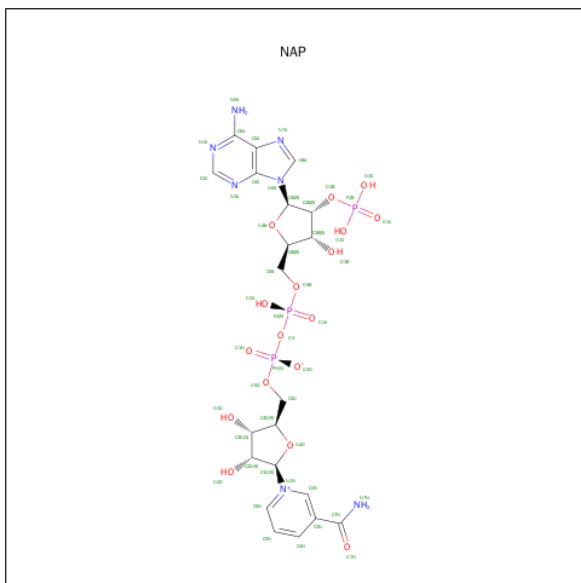
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Na 1 1	0	0
2	A	1	Total Na 1 1	0	0
2	D	1	Total Na 1 1	0	0
2	C	1	Total Na 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	1	Total	Na	0	0
			1	1		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 3 1 2	0	0
4	B	1	Total C O 3 1 2	0	0
4	C	1	Total C O 3 1 2	0	0
4	D	1	Total C O 3 1 2	0	0
4	E	1	Total C O 3 1 2	0	0

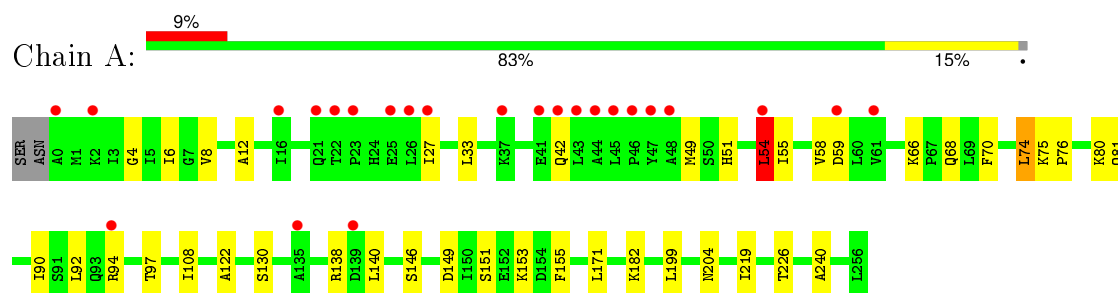
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	139	Total O 139 139	0	0
5	B	123	Total O 123 123	0	0
5	C	99	Total O 99 99	0	0
5	D	150	Total O 150 150	0	0
5	E	157	Total O 157 157	0	0

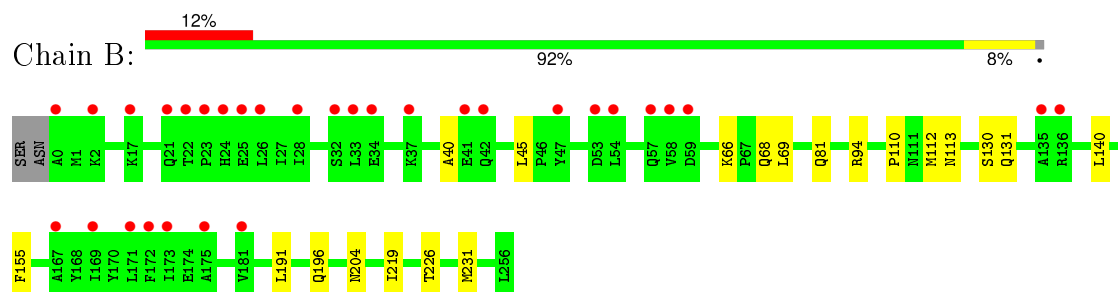
3 Residue-property plots [i](#)

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

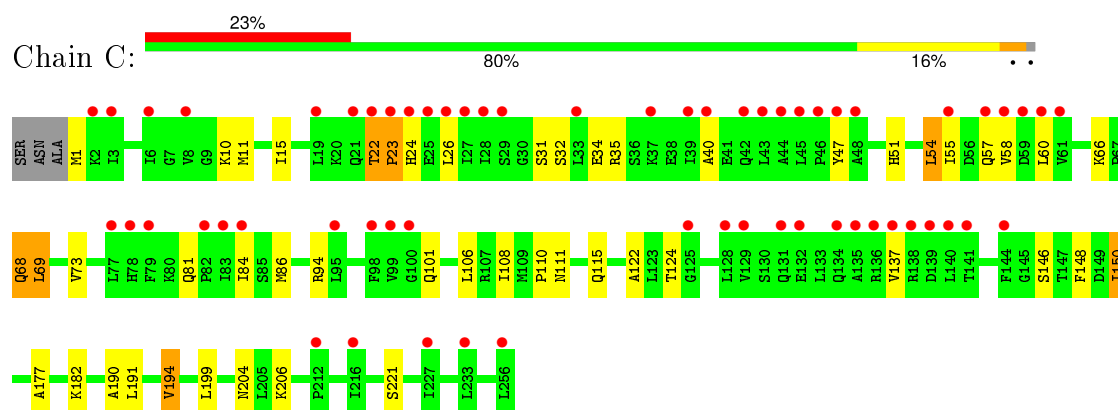
- Molecule 1: putative pyrroline carboxylate reductase



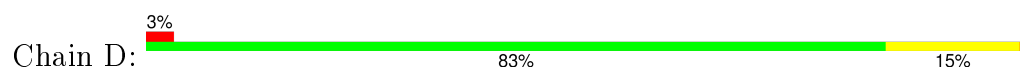
- Molecule 1: putative pyrroline carboxylate reductase

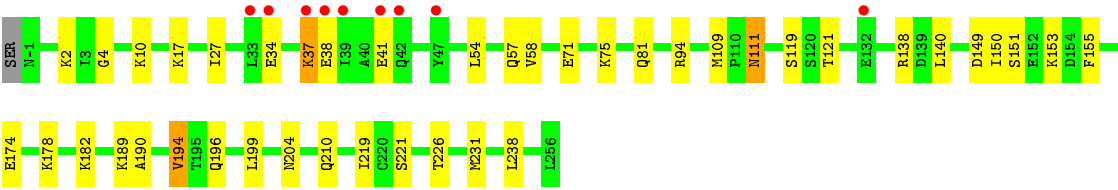


- Molecule 1: putative pyrroline carboxylate reductase

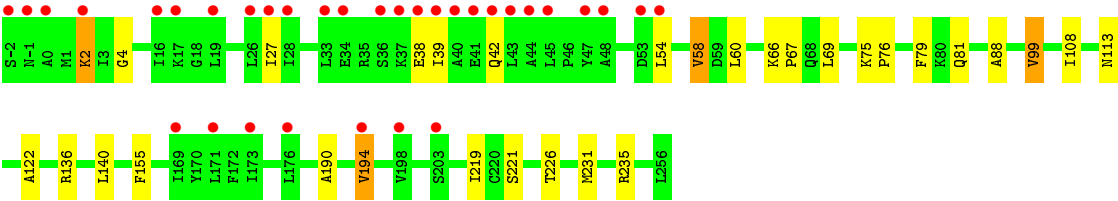
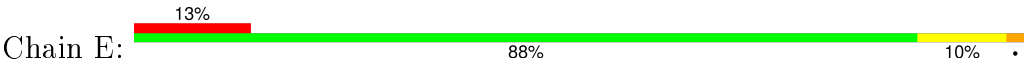


- Molecule 1: putative pyrroline carboxylate reductase





● Molecule 1: putative pyrroline carboxylate reductase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	171.63Å 109.65Å 84.03Å 90.00° 96.08° 90.00°	Depositor
Resolution (Å)	50.00 – 2.15 45.84 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-2.15) 99.0 (45.84-2.15)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.72 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.173 , 0.210 0.178 , 0.207	Depositor DCC
R_{free} test set	4155 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	37.0	Xtriage
Anisotropy	0.572	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 52.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 83006 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10547	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.43% 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: NA, FMT, NAP

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	0.62	0/1940	0.63	1/2612 (0.0%)
1	B	0.60	0/1940	0.60	1/2612 (0.0%)
1	C	0.60	0/1936	0.63	2/2608 (0.1%)
1	D	0.64	0/1945	0.60	0/2619
1	E	0.62	0/1954	0.63	1/2631 (0.0%)
All	All	0.62	0/9715	0.62	5/13082 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	LEU	CA-CB-CG	6.34	129.88	115.30
1	C	69	LEU	CA-CB-CG	5.71	128.42	115.30
1	E	54	LEU	CA-CB-CG	5.53	128.03	115.30
1	C	54	LEU	CA-CB-CG	5.24	127.35	115.30
1	B	191	LEU	CA-CB-CG	5.03	126.87	115.30

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	1921	0	2014	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1921	0	2014	9	0
1	C	1916	0	2009	32	0
1	D	1926	0	2016	27	0
1	E	1935	0	2025	16	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
3	A	48	0	25	0	0
3	B	48	0	25	1	0
3	C	48	0	25	1	0
3	D	48	0	25	2	0
3	E	48	0	25	0	0
4	A	3	0	1	0	0
4	B	3	0	1	0	0
4	C	3	0	1	0	0
4	D	3	0	1	0	0
4	E	3	0	1	0	0
5	A	139	0	0	1	0
5	B	123	0	0	2	0
5	C	99	0	0	1	0
5	D	150	0	0	5	0
5	E	157	0	0	4	0
All	All	10547	0	10208	104	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 5.

All (104) 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:D:138:ARG:HH22	1:D:149:ASP:HB2	1.38	0.86
1:E:88:ALA:HB3	5:E:1606:HOH:O	1.78	0.82
1:C:68:GLN:HE21	1:C:68:GLN:H	1.27	0.82
1:C:148:PHE:HB3	1:C:150:ILE:CD1	2.12	0.79
1:D:138:ARG:NH2	1:D:149:ASP:HB2	2.02	0.75
1:A:55:ILE:HG23	1:A:81:GLN:HE22	1.55	0.71
1:E:2:LYS:NZ	1:E:2:LYS:HB3	2.07	0.69
1:C:22:THR:N	1:C:23:PRO:HD2	2.09	0.68
1:C:32:SER:HB2	1:C:35:ARG:H	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:LYS:NZ	5:C:1538:HOH:O	2.26	0.67
1:D:178:LYS:NZ	5:D:1638:HOH:O	2.27	0.67
1:A:66:LYS:HB3	1:A:68:GLN:HE21	1.62	0.65
1:D:4:GLY:HA3	1:D:54:LEU:HD11	1.77	0.65
1:B:204:ASN:HD21	1:C:115:GLN:HE21	1.45	0.64
1:D:111:ASN:C	1:D:111:ASN:HD22	2.00	0.64
1:D:219:ILE:HG22	1:D:226:THR:HG21	1.82	0.61
1:C:22:THR:HG22	1:C:24:HIS:HD2	1.65	0.61
1:C:190:ALA:O	1:C:194:VAL:HG13	2.03	0.59
1:D:182:LYS:HD2	1:E:231:MSE:HG3	1.86	0.57
1:C:101:GLN:HG3	1:C:101:GLN:O	2.06	0.55
1:B:219:ILE:HG22	1:B:226:THR:HG21	1.88	0.55
1:E:67:PRO:HG3	5:E:1606:HOH:O	2.08	0.54
1:A:171:LEU:HD23	1:D:238:LEU:HD23	1.90	0.54
1:E:58:VAL:HG13	1:E:60:LEU:H	1.73	0.53
3:D:1503:NAP:O1A	5:D:1648:HOH:O	2.17	0.53
1:C:40:ALA:HB2	1:C:47:TYR:HB3	1.90	0.53
1:C:60:LEU:HD21	1:C:84:ILE:HD12	1.90	0.52
1:C:23:PRO:HA	1:C:24:HIS:HB2	1.92	0.51
1:D:94:ARG:HD3	5:D:1533:HOH:O	2.10	0.51
1:A:182:LYS:HD2	1:B:231:MSE:HG3	1.91	0.51
1:C:55:ILE:HG23	1:C:81:GLN:HE22	1.76	0.51
1:E:113:ASN:ND2	5:E:1576:HOH:O	2.43	0.51
1:D:138:ARG:HH22	1:D:149:ASP:CB	2.19	0.51
1:C:22:THR:N	1:C:23:PRO:CD	2.72	0.51
1:A:94:ARG:O	1:A:97:THR:HB	2.10	0.51
1:B:196:GLN:HE22	1:C:146:SER:HB2	1.75	0.51
1:E:136:ARG:NH2	5:E:1621:HOH:O	2.38	0.50
1:C:1:MSE:HB3	1:C:24:HIS:CE1	2.47	0.49
1:D:151:SER:OG	1:D:153:LYS:HG2	2.12	0.49
1:B:66:LYS:HE3	1:B:68:GLN:HB2	1.94	0.49
1:A:138:ARG:NH1	1:A:149:ASP:OD2	2.46	0.49
1:A:70:PHE:O	1:A:74:LEU:HB2	2.13	0.49
1:D:111:ASN:HD21	1:D:119:SER:HA	1.78	0.49
1:B:66:LYS:HE2	1:B:69:LEU:HD13	1.95	0.48
1:A:66:LYS:HB3	1:A:68:GLN:NE2	2.29	0.47
1:E:4:GLY:HA2	1:E:27:ILE:O	2.14	0.47
1:E:190:ALA:O	1:E:194:VAL:HG13	2.14	0.47
1:D:174:GLU:OE2	1:D:178:LYS:HE3	2.14	0.47
1:E:79:PHE:CD1	1:E:99:VAL:HG22	2.49	0.47
1:A:199:LEU:HD12	1:D:199:LEU:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:GLN:H	1:C:68:GLN:NE2	2.06	0.46
1:A:55:ILE:O	1:A:81:GLN:NE2	2.49	0.46
1:A:58:VAL:O	1:A:81:GLN:HG2	2.15	0.46
1:A:59:ASP:O	1:A:81:GLN:HB3	2.17	0.45
1:C:182:LYS:HD2	1:D:231:MSE:HG3	1.98	0.45
1:C:22:THR:CG2	1:C:24:HIS:HD2	2.27	0.45
1:D:37:LYS:HD2	1:D:38:GLU:N	2.32	0.45
1:D:4:GLY:CA	1:D:54:LEU:HD11	2.47	0.44
1:A:6:ILE:HG23	1:A:51:HIS:CE1	2.53	0.44
1:C:148:PHE:HB3	1:C:150:ILE:HD12	1.96	0.44
1:A:138:ARG:HH12	1:A:149:ASP:CG	2.21	0.44
3:D:1503:NAP:H1B	5:D:1517:HOH:O	2.18	0.44
1:C:51:HIS:O	1:C:54:LEU:HB3	2.18	0.43
1:A:75:LYS:N	1:A:76:PRO:HD2	2.34	0.43
1:C:15:ILE:HD12	1:C:86:MSE:CE	2.48	0.43
1:E:38:GLU:O	1:E:42:GLN:HG2	2.18	0.43
1:C:106:LEU:HD13	1:C:137:VAL:HG21	2.00	0.43
1:E:219:ILE:HG22	1:E:226:THR:HG21	2.01	0.43
1:A:33:LEU:HD21	1:A:49:MSE:HA	2.01	0.43
1:A:240:ALA:CB	1:E:235:ARG:HA	2.49	0.43
1:D:190:ALA:O	1:D:194:VAL:HG13	2.19	0.43
1:B:110:PRO:O	3:B:1501:NAP:H5N	2.19	0.42
1:E:108:ILE:HA	1:E:122:ALA:O	2.19	0.42
1:D:111:ASN:C	1:D:111:ASN:ND2	2.71	0.42
1:C:66:LYS:HB3	1:C:68:GLN:NE2	2.34	0.42
1:A:138:ARG:NH1	1:A:149:ASP:CG	2.73	0.42
1:A:108:ILE:HA	1:A:122:ALA:O	2.20	0.42
1:D:27:ILE:HG23	1:D:54:LEU:CD1	2.50	0.41
1:D:189:LYS:HA	1:D:189:LYS:HD3	1.88	0.41
1:A:51:HIS:O	1:A:54:LEU:HB3	2.19	0.41
1:B:40:ALA:HB1	1:B:45:LEU:O	2.21	0.41
1:E:66:LYS:HB2	1:E:67:PRO:HD2	2.02	0.41
1:C:15:ILE:HD12	1:C:86:MSE:HE1	2.01	0.41
1:C:110:PRO:O	3:C:1502:NAP:H5N	2.20	0.41
1:D:109:MSE:O	1:D:121:THR:HA	2.21	0.41
1:D:210:GLN:NE2	5:D:1644:HOH:O	2.50	0.41
1:A:219:ILE:HG22	1:A:226:THR:HG21	2.02	0.41
1:A:151:SER:OG	1:A:153:LYS:HG2	2.20	0.41
1:C:108:ILE:HA	1:C:122:ALA:O	2.21	0.41
1:A:8:VAL:HA	1:A:12:ALA:HB3	2.03	0.41
1:B:113:ASN:ND2	5:B:1556:HOH:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:MSE:HE1	1:C:111:ASN:O	2.21	0.41
1:C:23:PRO:HA	1:C:24:HIS:C	2.40	0.41
5:B:1603:HOH:O	1:C:10:LYS:HG3	2.20	0.41
1:A:4:GLY:HA2	1:A:27:ILE:O	2.20	0.41
1:A:42:GLN:NE2	5:A:1576:HOH:O	2.38	0.41
1:A:92:LEU:HA	1:A:92:LEU:HD23	1.97	0.41
1:D:2:LYS:NZ	1:D:57:GLN:HE21	2.19	0.40
1:C:22:THR:HG22	1:C:24:HIS:CD2	2.50	0.40
1:D:71:GLU:HG3	1:D:75:LYS:HD2	2.02	0.40
1:E:75:LYS:N	1:E:76:PRO:HD2	2.37	0.40
1:C:177:ALA:CB	1:C:191:LEU:HD13	2.51	0.40
1:D:34:GLU:O	1:D:38:GLU:HG3	2.21	0.40
1:A:146:SER:HB2	1:D:196:GLN:HE22	1.85	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	255/259 (98%)	250 (98%)	5 (2%)	0	100	100
1	B	255/259 (98%)	252 (99%)	3 (1%)	0	100	100
1	C	254/259 (98%)	244 (96%)	9 (4%)	1 (0%)	39	34
1	D	256/259 (99%)	253 (99%)	3 (1%)	0	100	100
1	E	257/259 (99%)	254 (99%)	3 (1%)	0	100	100
All	All	1277/1295 (99%)	1253 (98%)	23 (2%)	1 (0%)	56	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	23	PRO

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	212/207 (102%)	204 (96%)	8 (4%)	40	37
1	B	212/207 (102%)	205 (97%)	7 (3%)	45	44
1	C	212/207 (102%)	196 (92%)	16 (8%)	17	10
1	D	212/207 (102%)	199 (94%)	13 (6%)	23	17
1	E	214/207 (103%)	204 (95%)	10 (5%)	32	28
All	All	1062/1035 (103%)	1008 (95%)	54 (5%)	29	24

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LEU
1	A	74	LEU
1	A	80	LYS
1	A	90	ILE
1	A	130	SER
1	A	140	LEU
1	A	155	PHE
1	A	204	ASN
1	B	81	GLN
1	B	94	ARG
1	B	112	MSE
1	B	130	SER
1	B	131	GLN
1	B	140	LEU
1	B	155	PHE
1	C	22	THR
1	C	26	LEU
1	C	31	SER
1	C	34	GLU
1	C	57	GLN
1	C	58	VAL
1	C	68	GLN
1	C	69	LEU

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Mol	Chain	Res	Type
1	C	73	VAL
1	C	94	ARG
1	C	124	THR
1	C	150	ILE
1	C	194	VAL
1	C	199	LEU
1	C	204	ASN
1	C	221	SER
1	D	10	LYS
1	D	17	LYS
1	D	37	LYS
1	D	41	GLU
1	D	58	VAL
1	D	81	GLN
1	D	111	ASN
1	D	140	LEU
1	D	150	ILE
1	D	155	PHE
1	D	194	VAL
1	D	204	ASN
1	D	221	SER
1	E	2	LYS
1	E	39	ILE
1	E	58	VAL
1	E	69	LEU
1	E	81	GLN
1	E	99	VAL
1	E	140	LEU
1	E	155	PHE
1	E	194	VAL
1	E	221	SER

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	68	GLN
1	A	101	GLN
1	A	196	GLN
1	A	204	ASN
1	B	113	ASN
1	B	115	GLN
1	B	131	GLN

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Mol	Chain	Res	Type
1	B	196	GLN
1	C	21	GLN
1	C	68	GLN
1	C	113	ASN
1	C	115	GLN
1	C	196	GLN
1	C	204	ASN
1	D	21	GLN
1	D	57	GLN
1	D	111	ASN
1	D	115	GLN
1	D	196	GLN
1	D	204	ASN
1	E	113	ASN
1	E	196	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 5 are monoatomic - leaving 10 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	NAP	A	1500	-	42,52,52	1.53	3 (7%)	54,80,80	2.01	8 (14%)
4	FMT	A	1508	-	0,2,2	0.00	-	0,1,1	0.00	-
3	NAP	B	1501	-	42,52,52	1.60	3 (7%)	54,80,80	1.98	6 (11%)
4	FMT	B	1509	-	0,2,2	0.00	-	0,1,1	0.00	-
3	NAP	C	1502	-	42,52,52	1.62	3 (7%)	54,80,80	1.85	5 (9%)
4	FMT	C	1510	-	0,2,2	0.00	-	0,1,1	0.00	-
3	NAP	D	1503	-	42,52,52	1.61	3 (7%)	54,80,80	1.94	6 (11%)
4	FMT	D	1511	-	0,2,2	0.00	-	0,1,1	0.00	-
3	NAP	E	1504	-	42,52,52	1.59	3 (7%)	54,80,80	1.99	5 (9%)
4	FMT	E	1512	-	0,2,2	0.00	-	0,1,1	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	NAP	A	1500	-	-	0/27/67/67	0/5/5/5
4	FMT	A	1508	-	-	0/0/0/0	0/0/0/0
3	NAP	B	1501	-	-	0/27/67/67	0/5/5/5
4	FMT	B	1509	-	-	0/0/0/0	0/0/0/0
3	NAP	C	1502	-	-	0/27/67/67	0/5/5/5
4	FMT	C	1510	-	-	0/0/0/0	0/0/0/0
3	NAP	D	1503	-	-	0/27/67/67	0/5/5/5
4	FMT	D	1511	-	-	0/0/0/0	0/0/0/0
3	NAP	E	1504	-	-	0/27/67/67	0/5/5/5
4	FMT	E	1512	-	-	0/0/0/0	0/0/0/0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1503	NAP	C2A-N1A	2.52	1.38	1.33
3	E	1504	NAP	C2A-N1A	2.61	1.38	1.33
3	A	1500	NAP	C2A-N1A	2.66	1.39	1.33
3	C	1502	NAP	C2A-N1A	2.69	1.39	1.33
3	B	1501	NAP	C2A-N1A	2.83	1.39	1.33
3	E	1504	NAP	C2A-N3A	3.53	1.38	1.32
3	B	1501	NAP	C2A-N3A	3.73	1.38	1.32
3	C	1502	NAP	C2A-N3A	3.82	1.38	1.32
3	A	1500	NAP	C2A-N3A	3.93	1.39	1.32
3	D	1503	NAP	C2A-N3A	3.96	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1500	NAP	O7N-C7N	7.25	1.39	1.24
3	B	1501	NAP	O7N-C7N	7.94	1.41	1.24
3	D	1503	NAP	O7N-C7N	8.05	1.41	1.24
3	E	1504	NAP	O7N-C7N	8.08	1.41	1.24
3	C	1502	NAP	O7N-C7N	8.26	1.41	1.24

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1504	NAP	N3A-C2A-N1A	-11.69	119.94	128.89
3	B	1501	NAP	N3A-C2A-N1A	-11.45	120.13	128.89
3	D	1503	NAP	N3A-C2A-N1A	-11.43	120.14	128.89
3	A	1500	NAP	N3A-C2A-N1A	-11.19	120.33	128.89
3	C	1502	NAP	N3A-C2A-N1A	-10.73	120.67	128.89
3	B	1501	NAP	PN-O3-PA	-3.57	122.72	132.73
3	E	1504	NAP	PN-O3-PA	-3.09	124.06	132.73
3	D	1503	NAP	PN-O3-PA	-3.02	124.25	132.73
3	C	1502	NAP	PN-O3-PA	-2.96	124.40	132.73
3	A	1500	NAP	O7N-C7N-C3N	-2.90	116.42	119.59
3	B	1501	NAP	O7N-C7N-C3N	-2.80	116.53	119.59
3	A	1500	NAP	PN-O3-PA	-2.61	125.40	132.73
3	A	1500	NAP	C1B-N9A-C4A	-2.61	123.00	126.94
3	E	1504	NAP	O7N-C7N-C3N	-2.54	116.82	119.59
3	A	1500	NAP	O4D-C1D-N1N	-2.37	105.53	108.13
3	A	1500	NAP	O3D-C3D-C4D	-2.10	104.75	111.05
3	D	1503	NAP	O7N-C7N-C3N	-2.07	117.32	119.59
3	C	1502	NAP	C4A-C5A-N7A	-2.06	107.59	109.48
3	D	1503	NAP	C4A-C5A-N7A	-2.03	107.61	109.48
3	B	1501	NAP	O4D-C1D-N1N	2.10	110.43	108.13
3	C	1502	NAP	C3N-C7N-N7N	2.26	120.29	117.82
3	E	1504	NAP	C3N-C7N-N7N	2.75	120.83	117.82
3	D	1503	NAP	C3N-C7N-N7N	2.93	121.02	117.82
3	A	1500	NAP	O4B-C1B-N9A	2.93	114.23	108.10
3	D	1503	NAP	O4B-C1B-N9A	3.04	114.47	108.10
3	B	1501	NAP	O4B-C1B-N9A	3.33	115.07	108.10
3	E	1504	NAP	O4B-C1B-N9A	3.36	115.14	108.10
3	C	1502	NAP	O4B-C1B-N9A	3.62	115.67	108.10
3	B	1501	NAP	C3N-C7N-N7N	3.72	121.89	117.82
3	A	1500	NAP	C3N-C7N-N7N	3.95	122.14	117.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1501	NAP	1	0
3	C	1502	NAP	1	0
3	D	1503	NAP	2	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	250/259 (96%)	0.64	24 (9%) 10 16	29, 41, 58, 67	1 (0%)
1	B	250/259 (96%)	0.77	31 (12%) 5 9	30, 43, 63, 70	1 (0%)
1	C	249/259 (96%)	1.24	60 (24%) 1 2	30, 50, 84, 89	0
1	D	251/259 (96%)	0.46	9 (3%) 46 57	28, 41, 57, 67	2 (0%)
1	E	252/259 (97%)	0.81	33 (13%) 5 8	28, 40, 65, 71	2 (0%)
All	All	1252/1295 (96%)	0.79	157 (12%) 5 9	28, 42, 70, 89	6 (0%)

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	33	LEU	6.6
1	C	45	LEU	6.4
1	E	27	ILE	6.1
1	C	22	THR	5.8
1	C	60	LEU	5.7
1	E	39	ILE	5.3
1	A	48	ALA	5.0
1	B	0	ALA	4.8
1	E	37	LYS	4.7
1	C	26	LEU	4.5
1	E	45	LEU	4.5
1	C	58	VAL	4.5
1	A	22	THR	4.5
1	B	22	THR	4.4
1	C	136	ARG	4.3
1	C	6	ILE	4.3
1	C	132	GLU	4.2
1	C	46	PRO	4.2
1	C	129	VAL	4.2
1	A	47	TYR	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	0	ALA	4.1
1	B	28	ILE	4.0
1	E	48	ALA	3.9
1	C	19	LEU	3.9
1	C	43	LEU	3.9
1	C	48	ALA	3.9
1	E	33	LEU	3.9
1	E	47	TYR	3.9
1	A	23	PRO	3.8
1	D	37	LYS	3.8
1	C	47	TYR	3.7
1	C	24	HIS	3.7
1	C	27	ILE	3.7
1	A	45	LEU	3.7
1	A	27	ILE	3.7
1	C	128	LEU	3.7
1	C	131	GLN	3.6
1	B	37	LYS	3.6
1	C	37	LYS	3.6
1	B	54	LEU	3.6
1	B	32	SER	3.6
1	B	47	TYR	3.5
1	C	42	GLN	3.5
1	E	26	LEU	3.4
1	C	23	PRO	3.4
1	E	42	GLN	3.4
1	D	39	ILE	3.4
1	B	58	VAL	3.4
1	E	44	ALA	3.4
1	E	0	ALA	3.3
1	C	25	GLU	3.3
1	C	139	ASP	3.3
1	C	28	ILE	3.3
1	A	43	LEU	3.3
1	C	55	ILE	3.2
1	C	84	ILE	3.2
1	D	47	TYR	3.2
1	C	59	ASP	3.2
1	E	-2	SER	3.2
1	C	39	ILE	3.1
1	A	26	LEU	3.1
1	D	33	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	2	LYS	3.1
1	A	42	GLN	3.0
1	C	79	PHE	3.0
1	B	171	LEU	3.0
1	C	137	VAL	2.9
1	E	173	ILE	2.9
1	C	216	ILE	2.9
1	C	77	LEU	2.9
1	A	54	LEU	2.9
1	A	25	GLU	2.8
1	E	203	SER	2.8
1	A	135	ALA	2.8
1	E	16	ILE	2.8
1	A	59	ASP	2.8
1	A	21	GLN	2.7
1	B	41	GLU	2.7
1	C	44	ALA	2.7
1	C	40	ALA	2.7
1	B	57	GLN	2.7
1	C	82	PRO	2.7
1	B	33	LEU	2.7
1	C	95	LEU	2.7
1	E	28	ILE	2.7
1	D	41	GLU	2.7
1	E	41	GLU	2.6
1	C	98	PHE	2.6
1	A	37	LYS	2.6
1	B	23	PRO	2.6
1	C	29	SER	2.6
1	C	134	GLN	2.6
1	E	38	GLU	2.6
1	E	40	ALA	2.6
1	C	21	GLN	2.6
1	E	53	ASP	2.6
1	A	16	ILE	2.5
1	B	2	LYS	2.5
1	D	34	GLU	2.5
1	C	100	GLY	2.5
1	E	-1	ASN	2.5
1	E	171	LEU	2.5
1	B	181	VAL	2.5
1	B	42	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	175	ALA	2.5
1	B	53	ASP	2.5
1	B	169	ILE	2.5
1	C	138	ARG	2.5
1	E	17	LYS	2.4
1	D	42	GLN	2.4
1	A	2	LYS	2.4
1	E	54	LEU	2.4
1	B	25	GLU	2.3
1	C	141	THR	2.3
1	C	57	GLN	2.3
1	B	173	ILE	2.3
1	C	3	ILE	2.3
1	C	83	ILE	2.3
1	E	36	SER	2.3
1	C	140	LEU	2.3
1	E	19	LEU	2.3
1	C	78	HIS	2.3
1	B	26	LEU	2.3
1	B	167	ALA	2.3
1	D	132	GLU	2.3
1	A	46	PRO	2.2
1	C	99	VAL	2.2
1	B	24	HIS	2.2
1	B	21	GLN	2.2
1	E	34	GLU	2.2
1	C	144	PHE	2.2
1	A	44	ALA	2.2
1	C	135	ALA	2.2
1	C	233	LEU	2.2
1	C	256	LEU	2.2
1	B	136	ARG	2.2
1	C	125	GLY	2.2
1	A	41	GLU	2.1
1	B	17	LYS	2.1
1	E	194	VAL	2.1
1	C	8	VAL	2.1
1	B	59	ASP	2.1
1	C	2	LYS	2.1
1	E	169	ILE	2.1
1	E	176	LEU	2.1
1	B	34	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	38	GLU	2.1
1	C	61	VAL	2.1
1	E	198	VAL	2.1
1	A	94	ARG	2.0
1	B	172	PHE	2.0
1	C	227	ILE	2.0
1	E	43	LEU	2.0
1	A	139	ASP	2.0
1	B	135	ALA	2.0
1	A	61	VAL	2.0
1	C	212	PRO	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(Å ²)	Q<0.9
3	NAP	D	1503	48/48	0.93	0.14	0.44	49,60,69,71	0
2	NA	D	1260	1/1	0.94	0.16	0.35	37,37,37,37	0
3	NAP	B	1501	48/48	0.88	0.15	-0.17	52,75,81,83	0
3	NAP	E	1504	48/48	0.91	0.13	-0.37	47,71,80,81	0
3	NAP	C	1502	48/48	0.93	0.13	-0.50	51,66,78,78	0
4	FMT	B	1509	3/3	0.82	0.12	-0.67	59,59,60,61	0
4	FMT	D	1511	3/3	0.94	0.10	-0.83	64,64,64,65	0
4	FMT	C	1510	3/3	0.87	0.12	-0.88	66,66,66,66	0
3	NAP	A	1500	48/48	0.94	0.11	-1.18	41,53,58,60	0
2	NA	A	1257	1/1	0.97	0.06	-1.41	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	FMT	E	1512	3/3	0.93	0.10	-1.63	64,64,65,65	0
2	NA	C	1259	1/1	0.94	0.07	-1.91	48,48,48,48	0
2	NA	E	1261	1/1	0.98	0.07	-2.55	40,40,40,40	0
2	NA	B	1258	1/1	0.90	0.05	-3.29	46,46,46,46	0
4	FMT	A	1508	3/3	0.90	0.16	-	62,62,62,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.