Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:01 AM GMT

PDB ID	:	3D03
Title	:	1.9A structure of Glycerophoshphodiesterase (GpdQ) from Enterobacter aerogenes
Authors	:	Hadler, K.S.; Tanifum, E.; Yip, S.H.-C.; Miti, N.; Guddat, L.W.; Jackson, C.J.; Gahan, L.R.; Carr, P.D.; Nguyen, K.; Ollis, D.L.; Hengge, A.C.; Larrabee, J.A.; Schenk, G.
Deposited on	:	2008-04-30
Resolution	:	1.90 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

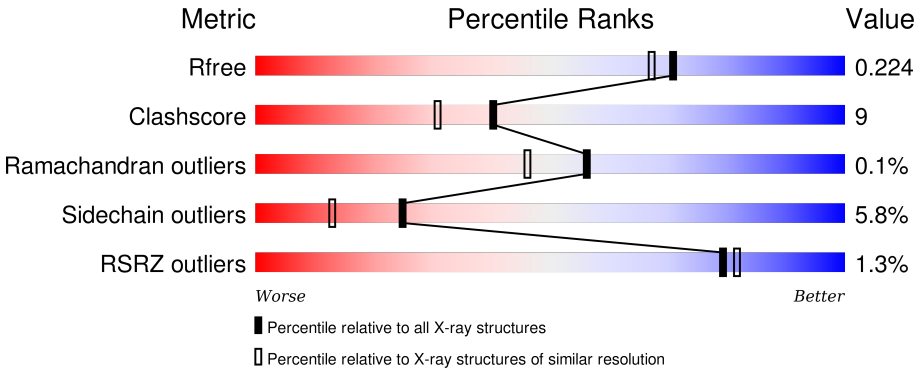
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.90 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}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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 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 <=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	274	85% 12%
1	B	274	88% 9%
1	C	274	2% 84% 13%
1	D	274	81% 16%
1	E	274	85% 11%

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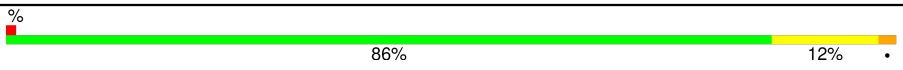
Mol	Chain	Length	Quality of chain
1	F	274	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13904 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 Phosphohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2163	1364	378	407	14			
1	B	271	Total	C	N	O	S	0	0	0
			2133	1348	372	399	14			
1	C	271	Total	C	N	O	S	0	0	0
			2133	1348	372	399	14			
1	D	271	Total	C	N	O	S	0	0	0
			2133	1348	372	399	14			
1	E	271	Total	C	N	O	S	0	0	0
			2133	1348	372	399	14			
1	F	274	Total	C	N	O	S	0	0	0
			2163	1364	378	407	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	224	ALA	GLU	SEE REMARK 999	UNP Q6XBH1
A	227	ASP	ARG	SEE REMARK 999	UNP Q6XBH1
B	224	ALA	GLU	SEE REMARK 999	UNP Q6XBH1
B	227	ASP	ARG	SEE REMARK 999	UNP Q6XBH1
C	224	ALA	GLU	SEE REMARK 999	UNP Q6XBH1
C	227	ASP	ARG	SEE REMARK 999	UNP Q6XBH1
D	224	ALA	GLU	SEE REMARK 999	UNP Q6XBH1
D	227	ASP	ARG	SEE REMARK 999	UNP Q6XBH1
E	224	ALA	GLU	SEE REMARK 999	UNP Q6XBH1
E	227	ASP	ARG	SEE REMARK 999	UNP Q6XBH1
F	224	ALA	GLU	SEE REMARK 999	UNP Q6XBH1
F	227	ASP	ARG	SEE REMARK 999	UNP Q6XBH1

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

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

- Molecule 3 is water.

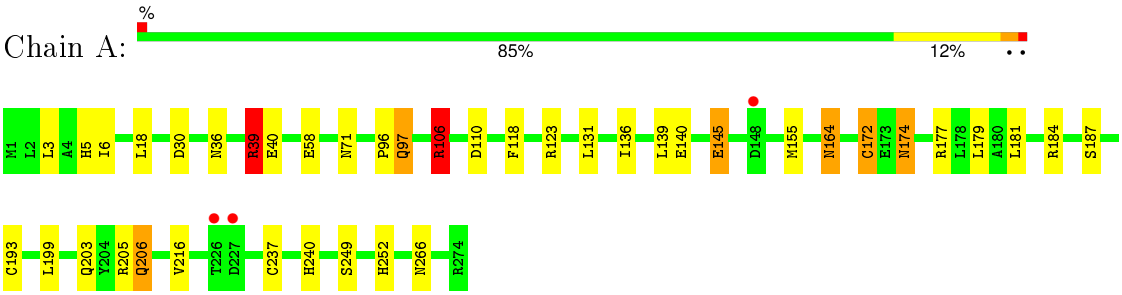
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	179	Total O 179 179	0	0
3	B	178	Total O 178 178	0	0
3	C	178	Total O 178 178	0	0
3	D	181	Total O 181 181	0	0
3	E	139	Total O 139 139	0	0
3	F	179	Total O 179 179	0	0

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.

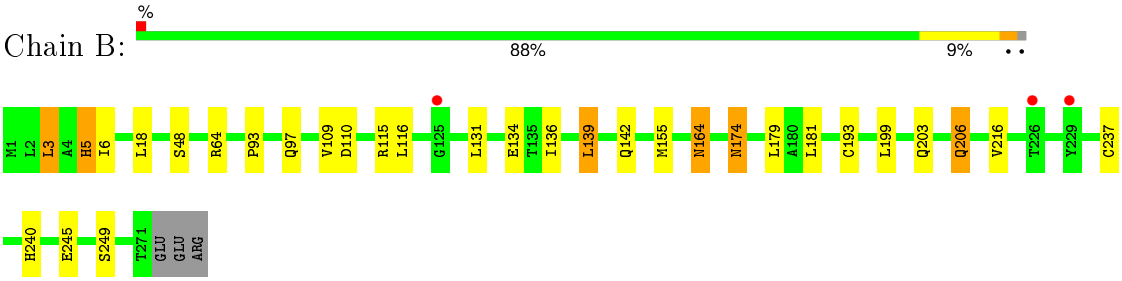
- Molecule 1: Phosphohydrolase

Chain A:



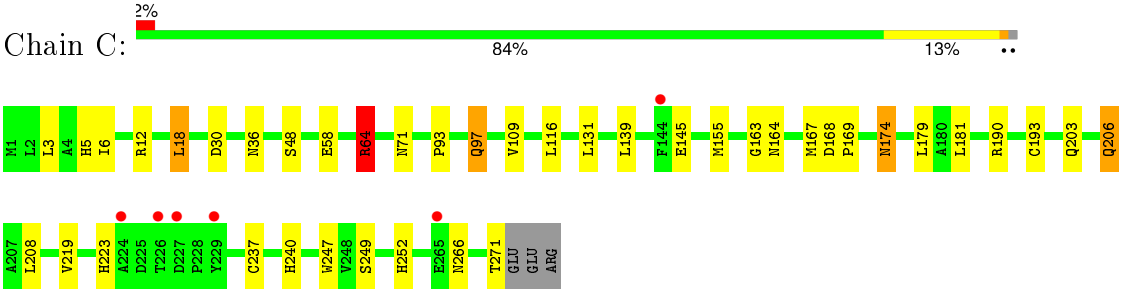
- Molecule 1: Phosphohydrolase

Chain B:



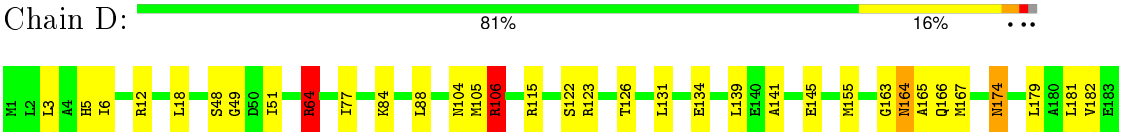
- Molecule 1: Phosphohydrolase

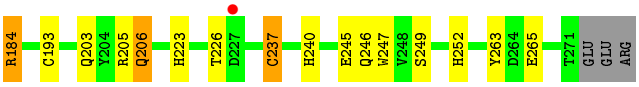
Chain C:



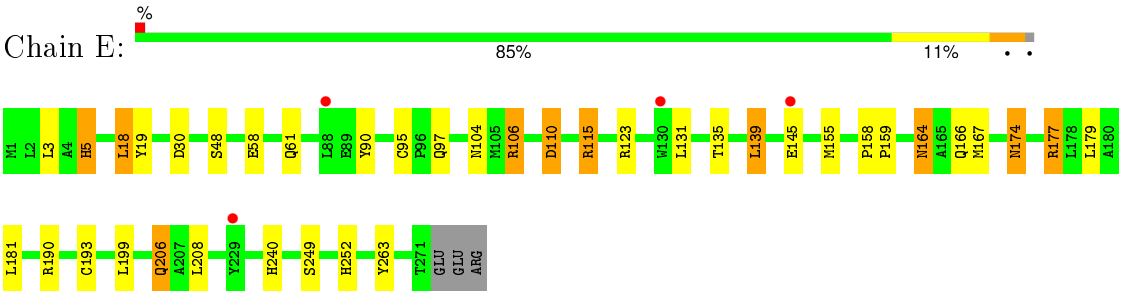
- Molecule 1: Phosphohydrolase

Chain D:

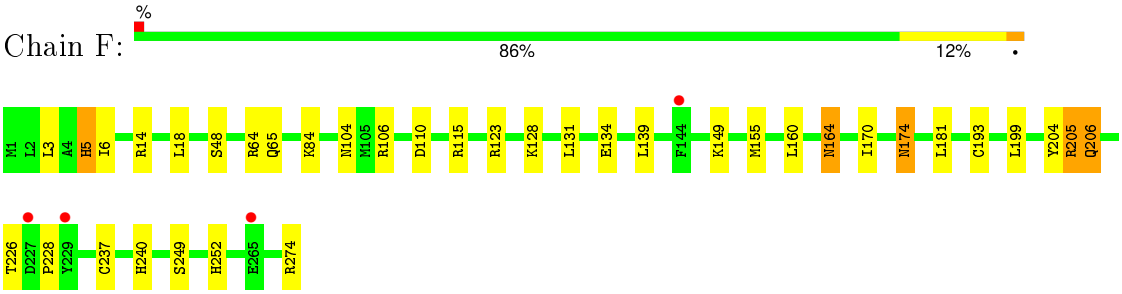




• Molecule 1: Phosphohydrolase



• Molecule 1: Phosphohydrolase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	94.97Å 133.84Å 168.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.27 – 1.90 43.26 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.7 (43.27-1.90) 96.7 (43.26-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.184 , 0.223 0.187 , 0.224	Depositor DCC
R_{free} test set	8219 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	16.5	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 37.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 163720 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13904	wwPDB-VP
Average B, all atoms (Å^2)	8.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.81	1/2222 (0.0%)	0.82	3/3029 (0.1%)
1	B	0.79	1/2192 (0.0%)	0.75	2/2991 (0.1%)
1	C	0.79	0/2192	0.79	4/2991 (0.1%)
1	D	0.80	1/2192 (0.0%)	0.81	4/2991 (0.1%)
1	E	0.68	0/2192	0.73	2/2991 (0.1%)
1	F	0.78	0/2222	0.78	1/3029 (0.0%)
All	All	0.77	3/13212 (0.0%)	0.78	16/18022 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	134	GLU	CG-CD	5.30	1.59	1.51
1	D	237	CYS	CB-SG	-5.15	1.73	1.81
1	A	172	CYS	CB-SG	-5.01	1.73	1.81

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	106	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	A	39	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	E	139	LEU	CA-CB-CG	5.88	128.83	115.30
1	A	30	ASP	CB-CG-OD1	5.87	123.59	118.30
1	C	12	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	D	12	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	C	64	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	D	64	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	C	30	ASP	CB-CG-OD1	5.61	123.35	118.30
1	C	18	LEU	CB-CG-CD2	5.52	120.38	111.00
1	B	139	LEU	CA-CB-CG	5.33	127.56	115.30
1	F	84	LYS	CD-CE-NZ	-5.32	99.47	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	12	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	B	3	LEU	CB-CG-CD1	5.16	119.78	111.00
1	E	30	ASP	CB-CG-OD1	5.13	122.92	118.30
1	A	106	ARG	NE-CZ-NH2	-5.13	117.74	120.30

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	2163	0	2071	48	0
1	B	2133	0	2046	31	0
1	C	2133	0	2046	36	0
1	D	2133	0	2046	44	0
1	E	2133	0	2046	44	0
1	F	2163	0	2071	38	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	179	0	0	4	0
3	B	178	0	0	1	0
3	C	178	0	0	6	0
3	D	181	0	0	5	0
3	E	139	0	0	2	0
3	F	179	0	0	6	0
All	All	13904	0	12326	218	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 9.

All (218) 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:199:LEU:CD2	1:B:199:LEU:CD2	2.26	1.14
1:A:39:ARG:HD3	1:A:39:ARG:N	1.56	1.12
1:A:199:LEU:HD21	1:B:199:LEU:CD2	1.87	1.01
1:B:97:GLN:HG3	3:B:2124:HOH:O	1.60	1.01
1:E:106:ARG:HG3	1:E:106:ARG:HH11	0.87	1.01
1:A:39:ARG:H	1:A:39:ARG:HD3	1.17	0.98
1:E:106:ARG:CG	1:E:106:ARG:HH11	1.77	0.96
1:E:177:ARG:HH11	1:E:177:ARG:HG2	1.31	0.96
1:C:266:ASN:HB2	3:C:2129:HOH:O	1.65	0.95
1:F:131:LEU:H	1:F:174:ASN:HD21	1.10	0.95
1:E:106:ARG:NH1	1:E:106:ARG:HG3	1.69	0.94
1:E:95:CYS:SG	1:E:97:GLN:NE2	2.40	0.94
1:B:131:LEU:H	1:B:174:ASN:HD21	1.14	0.94
1:A:199:LEU:CD2	1:B:199:LEU:HD21	1.98	0.93
1:A:199:LEU:HD21	1:B:199:LEU:HD21	1.51	0.93
1:E:199:LEU:CD2	1:F:199:LEU:HD21	1.99	0.92
1:E:199:LEU:HD23	1:F:199:LEU:CD2	2.00	0.91
1:E:199:LEU:CD2	1:F:199:LEU:CD2	2.49	0.91
1:F:104:ASN:HD22	1:F:106:ARG:HH22	1.06	0.91
1:A:39:ARG:CD	1:A:39:ARG:H	1.86	0.88
1:E:199:LEU:HD23	1:F:199:LEU:HD21	1.53	0.87
1:F:5:HIS:HD2	1:F:240:HIS:HE1	1.21	0.86
1:C:131:LEU:H	1:C:174:ASN:HD21	1.17	0.86
1:E:5:HIS:HD2	1:E:240:HIS:HE1	1.25	0.85
1:A:199:LEU:CD2	1:B:199:LEU:HD23	2.08	0.84
1:E:131:LEU:H	1:E:174:ASN:HD21	1.23	0.83
1:A:131:LEU:H	1:A:174:ASN:HD21	1.26	0.83
1:A:199:LEU:HD23	1:B:199:LEU:CD2	2.08	0.83
1:A:199:LEU:HD21	1:B:199:LEU:HD23	1.59	0.82
1:D:174:ASN:HD22	1:D:174:ASN:H	1.28	0.82
1:D:5:HIS:HD2	1:D:240:HIS:HE1	1.27	0.81
1:A:39:ARG:CD	1:A:39:ARG:N	2.42	0.81
1:C:36:ASN:HD21	1:C:71:ASN:H	1.29	0.80
1:E:5:HIS:CD2	1:E:240:HIS:HE1	1.99	0.80
1:D:131:LEU:H	1:D:174:ASN:HD21	1.29	0.80
1:B:5:HIS:HD2	1:B:240:HIS:HE1	1.28	0.79
1:F:5:HIS:CD2	1:F:240:HIS:HE1	2.01	0.79
1:A:266:ASN:HB2	3:A:2102:HOH:O	1.85	0.76
1:B:115:ARG:HH12	1:B:142:GLN:HE21	1.31	0.76
1:B:5:HIS:CD2	1:B:240:HIS:HE1	2.04	0.75
1:D:5:HIS:CD2	1:D:240:HIS:HE1	2.06	0.74
1:C:5:HIS:HD2	1:C:240:HIS:HE1	1.38	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:ASN:ND2	3:D:2097:HOH:O	2.23	0.70
1:D:64:ARG:HG3	1:D:64:ARG:HH11	1.57	0.70
1:F:104:ASN:HD22	1:F:106:ARG:NH2	1.86	0.70
1:E:61:GLN:HG2	3:E:2127:HOH:O	1.91	0.69
1:A:36:ASN:HD21	1:A:71:ASN:H	1.39	0.69
1:E:166:GLN:HG2	1:E:167:MET:CE	2.22	0.69
1:E:199:LEU:HD21	1:F:199:LEU:HD21	1.74	0.68
1:A:174:ASN:H	1:A:174:ASN:HD22	1.39	0.68
1:F:104:ASN:HD21	1:F:134:GLU:HG3	1.57	0.68
1:D:84:LYS:HE2	3:D:2137:HOH:O	1.92	0.68
1:D:184:ARG:HB3	1:D:184:ARG:HH11	1.58	0.68
1:C:252:HIS:HE1	3:C:2019:HOH:O	1.76	0.67
1:A:5:HIS:CD2	1:A:240:HIS:HE1	2.14	0.66
1:C:36:ASN:ND2	1:C:71:ASN:H	1.95	0.65
1:A:140:GLU:CD	1:A:184:ARG:HH22	2.00	0.65
1:F:115:ARG:NE	3:F:2084:HOH:O	2.30	0.64
1:A:145:GLU:HB3	3:A:2078:HOH:O	1.96	0.64
1:F:115:ARG:CD	3:F:2084:HOH:O	2.46	0.64
1:A:5:HIS:HD2	1:A:240:HIS:HE1	1.44	0.64
1:C:5:HIS:CD2	1:C:240:HIS:HE1	2.13	0.63
1:C:174:ASN:H	1:C:174:ASN:HD22	1.46	0.63
1:E:166:GLN:HG2	1:E:167:MET:HE3	1.81	0.63
1:C:240:HIS:HD2	1:C:249:SER:OG	1.82	0.62
1:E:177:ARG:HH11	1:E:177:ARG:CG	2.09	0.62
1:C:64:ARG:CD	3:C:2015:HOH:O	2.48	0.62
1:F:115:ARG:CZ	3:F:2084:HOH:O	2.48	0.61
1:B:115:ARG:HH22	1:B:142:GLN:HE22	1.48	0.61
1:A:131:LEU:HB3	1:A:136:ILE:HD11	1.83	0.61
1:A:39:ARG:H	1:A:39:ARG:HH11	1.47	0.60
1:F:5:HIS:HD2	1:F:240:HIS:CE1	2.12	0.60
1:E:199:LEU:HD21	1:F:199:LEU:CD2	2.30	0.60
1:C:167:MET:CE	1:C:219:VAL:HG11	2.31	0.60
1:F:128:LYS:HG2	1:F:170:ILE:HA	1.83	0.60
1:E:58:GLU:OE1	1:E:61:GLN:NE2	2.35	0.59
1:D:115:ARG:HH12	1:D:145:GLU:HG3	1.68	0.59
1:E:5:HIS:HD2	1:E:240:HIS:CE1	2.13	0.58
1:F:174:ASN:H	1:F:174:ASN:HD22	1.48	0.58
1:D:163:GLY:O	1:D:223:HIS:HD2	1.86	0.58
1:F:14:ARG:NH2	1:F:65:GLN:OE1	2.37	0.58
1:D:174:ASN:H	1:D:174:ASN:ND2	1.97	0.58
1:C:64:ARG:HH11	1:C:64:ARG:HG3	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:ASN:C	1:B:164:ASN:HD22	2.06	0.57
1:D:166:GLN:HG2	1:D:167:MET:CE	2.34	0.57
1:E:199:LEU:CD2	1:F:199:LEU:HD23	2.34	0.57
1:A:36:ASN:ND2	1:A:71:ASN:H	2.02	0.57
1:C:64:ARG:HH22	1:C:93:PRO:HG2	1.70	0.57
1:A:136:ILE:HD13	1:A:177:ARG:CZ	2.35	0.57
1:C:64:ARG:HD2	3:C:2015:HOH:O	2.02	0.57
1:A:39:ARG:NH1	1:A:39:ARG:H	2.03	0.56
1:E:106:ARG:N	1:E:106:ARG:HD2	2.20	0.56
1:D:164:ASN:C	1:D:164:ASN:HD22	2.07	0.56
1:A:39:ARG:HH11	1:A:39:ARG:N	2.03	0.56
1:D:64:ARG:HG3	1:D:64:ARG:NH1	2.20	0.56
1:E:104:ASN:HD22	1:E:106:ARG:HH21	1.55	0.55
1:A:58:GLU:CD	1:A:58:GLU:H	2.09	0.55
1:B:5:HIS:HD2	1:B:240:HIS:CE1	2.17	0.55
1:A:6:ILE:HG22	1:A:237:CYS:HB3	1.89	0.55
1:D:166:GLN:HG2	1:D:167:MET:HE3	1.89	0.55
1:D:104:ASN:ND2	1:D:106:ARG:HH22	2.05	0.55
1:E:61:GLN:HG3	1:E:90:TYR:CE2	2.42	0.54
1:E:58:GLU:HG3	1:F:274:ARG:HD2	1.89	0.54
1:B:115:ARG:HH12	1:B:142:GLN:NE2	2.04	0.54
1:A:199:LEU:HD23	1:B:199:LEU:HD21	1.74	0.54
1:E:174:ASN:H	1:E:174:ASN:HD22	1.54	0.54
1:A:136:ILE:HD13	1:A:177:ARG:NE	2.23	0.54
1:A:164:ASN:C	1:A:164:ASN:HD22	2.12	0.54
1:D:165:ALA:HB1	1:D:226:THR:HG22	1.90	0.53
1:B:174:ASN:HD22	1:B:174:ASN:H	1.57	0.53
1:F:155:MET:O	1:F:193:CYS:HA	2.08	0.53
1:A:155:MET:O	1:A:193:CYS:HA	2.09	0.53
1:E:106:ARG:NH1	1:E:106:ARG:CG	2.49	0.52
1:D:205:ARG:NH1	3:D:2163:HOH:O	2.36	0.52
1:A:96:PRO:HD2	1:A:97:GLN:HE22	1.75	0.52
1:C:167:MET:HE2	1:C:219:VAL:HG11	1.92	0.52
1:D:5:HIS:HE1	1:D:48:SER:OG	1.93	0.51
1:B:206:GLN:H	1:B:206:GLN:NE2	2.08	0.51
1:C:97:GLN:NE2	1:C:97:GLN:H	2.09	0.51
1:D:174:ASN:HD22	1:D:174:ASN:N	1.94	0.51
1:D:263:TYR:HE2	1:D:265:GLU:HG3	1.75	0.51
1:D:240:HIS:HD2	1:D:249:SER:OG	1.93	0.51
1:A:5:HIS:O	1:A:237:CYS:HB2	2.11	0.51
1:F:204:TYR:CE2	1:F:205:ARG:HD3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:177:ARG:NH1	1:E:177:ARG:HG2	2.11	0.51
1:F:5:HIS:HE1	1:F:48:SER:OG	1.94	0.51
1:C:155:MET:O	1:C:193:CYS:HA	2.11	0.51
1:B:64:ARG:HH22	1:B:93:PRO:HG2	1.75	0.51
1:D:5:HIS:HD2	1:D:240:HIS:CE1	2.17	0.50
1:B:240:HIS:HD2	1:B:249:SER:OG	1.94	0.50
1:F:115:ARG:HD2	3:F:2084:HOH:O	2.09	0.50
1:D:49:GLY:HA2	1:D:77:ILE:O	2.12	0.50
1:D:184:ARG:NH1	1:D:184:ARG:HB3	2.26	0.50
1:C:206:GLN:NE2	1:C:206:GLN:H	2.10	0.49
1:E:5:HIS:HE1	1:E:48:SER:OG	1.95	0.49
1:A:240:HIS:HD2	1:A:249:SER:OG	1.95	0.49
1:F:204:TYR:C	1:F:205:ARG:HG2	2.30	0.49
1:F:252:HIS:HE1	3:F:2070:HOH:O	1.95	0.49
1:A:206:GLN:NE2	1:A:206:GLN:H	2.11	0.48
1:D:206:GLN:NE2	1:D:206:GLN:H	2.10	0.48
1:F:104:ASN:ND2	1:F:106:ARG:HH22	1.91	0.48
1:D:134:GLU:CD	1:D:134:GLU:H	2.16	0.48
1:C:6:ILE:HG22	1:C:237:CYS:HB3	1.95	0.48
1:C:64:ARG:NH1	1:C:64:ARG:HG3	2.29	0.48
1:F:240:HIS:HD2	1:F:249:SER:OG	1.96	0.48
1:E:164:ASN:C	1:E:164:ASN:HD22	2.16	0.47
1:E:206:GLN:NE2	1:E:206:GLN:H	2.12	0.47
1:E:110:ASP:OD1	1:E:115:ARG:NH1	2.47	0.47
1:A:96:PRO:HD2	1:A:97:GLN:NE2	2.29	0.47
1:C:240:HIS:CD2	1:C:247:TRP:HE1	2.32	0.47
1:D:263:TYR:CE2	1:D:265:GLU:HG3	2.48	0.47
1:C:190:ARG:HD3	1:C:208:LEU:HB3	1.96	0.47
1:E:97:GLN:CD	1:E:97:GLN:H	2.18	0.47
1:C:271:THR:C	3:C:2052:HOH:O	2.52	0.47
1:D:174:ASN:N	1:D:174:ASN:ND2	2.61	0.47
1:A:203:GLN:HG3	1:B:203:GLN:HE22	1.80	0.47
1:A:252:HIS:HE1	3:A:2057:HOH:O	1.98	0.46
1:C:5:HIS:HE1	1:C:48:SER:OG	1.99	0.46
1:F:104:ASN:ND2	1:F:134:GLU:HG3	2.27	0.46
1:E:240:HIS:HD2	1:E:249:SER:OG	1.99	0.46
1:D:141:ALA:O	1:D:145:GLU:HB3	2.16	0.45
1:F:110:ASP:OD1	1:F:149:LYS:NZ	2.42	0.45
1:B:115:ARG:HH22	1:B:142:GLN:NE2	2.14	0.45
1:A:174:ASN:H	1:A:174:ASN:ND2	2.11	0.45
1:E:166:GLN:CG	1:E:167:MET:HE3	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:GLN:NE2	3:A:2033:HOH:O	2.50	0.45
1:D:84:LYS:NZ	1:D:122:SER:O	2.50	0.45
1:C:203:GLN:HE22	1:D:203:GLN:CG	2.29	0.45
1:B:5:HIS:HE1	1:B:48:SER:OG	2.00	0.45
1:B:109:VAL:HB	1:B:116:LEU:HB2	1.99	0.45
1:E:106:ARG:HH12	1:E:135:THR:HA	1.81	0.44
1:C:109:VAL:HB	1:C:116:LEU:HB2	1.99	0.44
1:C:174:ASN:HD22	1:C:174:ASN:N	2.09	0.44
1:C:64:ARG:NE	3:C:2015:HOH:O	2.50	0.44
1:A:199:LEU:HD23	1:B:199:LEU:HD22	1.92	0.44
1:A:39:ARG:HH11	1:A:40:GLU:H	1.66	0.44
1:C:58:GLU:H	1:C:58:GLU:CD	2.20	0.44
1:F:164:ASN:HD22	1:F:164:ASN:C	2.21	0.44
1:D:164:ASN:ND2	1:D:167:MET:H	2.16	0.44
1:D:6:ILE:HG22	1:D:237:CYS:HB3	1.98	0.44
1:E:263:TYR:HB3	1:F:228:PRO:HB2	2.00	0.44
1:C:167:MET:HE3	1:C:219:VAL:HG11	1.99	0.43
1:D:166:GLN:CG	1:D:167:MET:HE3	2.48	0.43
1:E:61:GLN:HG3	1:E:90:TYR:HE2	1.82	0.43
1:A:131:LEU:HB3	1:A:136:ILE:CD1	2.47	0.43
1:E:155:MET:O	1:E:193:CYS:HA	2.18	0.43
1:D:104:ASN:HD22	1:D:106:ARG:HH22	1.65	0.43
1:F:6:ILE:HG22	1:F:237:CYS:HB3	2.00	0.43
1:A:106:ARG:HB2	1:A:118:PHE:O	2.19	0.43
1:D:88:LEU:HD13	1:D:105:MET:SD	2.58	0.43
1:A:174:ASN:HD22	1:A:174:ASN:N	2.02	0.42
1:F:206:GLN:H	1:F:206:GLN:NE2	2.17	0.42
1:D:123:ARG:HD2	1:D:126:THR:CG2	2.49	0.42
1:E:252:HIS:HE1	3:E:2024:HOH:O	2.02	0.42
1:F:174:ASN:N	1:F:174:ASN:HD22	2.11	0.42
1:E:190:ARG:HD3	1:E:208:LEU:HB3	2.01	0.42
1:C:5:HIS:O	1:C:237:CYS:HB2	2.19	0.42
1:C:163:GLY:O	1:C:223:HIS:CD2	2.73	0.42
1:C:64:ARG:HH11	1:C:64:ARG:CG	2.32	0.42
1:D:246:GLN:NE2	3:D:2066:HOH:O	2.48	0.42
1:E:177:ARG:NH1	1:E:177:ARG:CG	2.75	0.42
1:A:131:LEU:CB	1:A:136:ILE:HD11	2.48	0.42
1:E:158:PRO:HA	1:E:159:PRO:HD3	1.70	0.41
1:E:18:LEU:HD13	1:E:19:TYR:CE2	2.55	0.41
1:C:168:ASP:N	1:C:169:PRO:CD	2.83	0.41
1:C:203:GLN:HE22	1:D:203:GLN:HG3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:MET:O	1:B:193:CYS:HA	2.20	0.41
1:D:64:ARG:CG	1:D:64:ARG:HH11	2.31	0.41
1:B:174:ASN:HD22	1:B:174:ASN:N	2.18	0.41
1:F:205:ARG:HB2	1:F:206:GLN:H	1.50	0.41
1:A:203:GLN:CG	1:B:203:GLN:HE22	2.33	0.41
1:F:64:ARG:NE	3:F:2170:HOH:O	2.46	0.41
1:D:252:HIS:HE1	3:D:2034:HOH:O	2.03	0.41
1:D:155:MET:O	1:D:193:CYS:HA	2.20	0.40
1:A:199:LEU:CD2	1:B:199:LEU:HD22	2.38	0.40
1:B:6:ILE:HG22	1:B:237:CYS:HB3	2.02	0.40
1:D:240:HIS:CD2	1:D:247:TRP:HE1	2.39	0.40
1:C:163:GLY:O	1:C:223:HIS:HD2	2.04	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	272/274 (99%)	262 (96%)	9 (3%)	1 (0%)	39	27
1	B	269/274 (98%)	263 (98%)	5 (2%)	1 (0%)	39	27
1	C	269/274 (98%)	261 (97%)	8 (3%)	0	100	100
1	D	269/274 (98%)	258 (96%)	11 (4%)	0	100	100
1	E	269/274 (98%)	260 (97%)	9 (3%)	0	100	100
1	F	272/274 (99%)	264 (97%)	8 (3%)	0	100	100
All	All	1620/1644 (98%)	1568 (97%)	50 (3%)	2 (0%)	56	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	216	VAL

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Mol	Chain	Res	Type
1	A	216	VAL

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	235/235 (100%)	218 (93%)	17 (7%)	18 7
1	B	232/235 (99%)	220 (95%)	12 (5%)	29 17
1	C	232/235 (99%)	221 (95%)	11 (5%)	32 20
1	D	232/235 (99%)	218 (94%)	14 (6%)	24 12
1	E	232/235 (99%)	217 (94%)	15 (6%)	21 10
1	F	235/235 (100%)	223 (95%)	12 (5%)	29 17
All	All	1398/1410 (99%)	1317 (94%)	81 (6%)	25 13

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	18	LEU
1	A	39	ARG
1	A	97	GLN
1	A	106	ARG
1	A	110	ASP
1	A	123	ARG
1	A	139	LEU
1	A	145	GLU
1	A	164	ASN
1	A	172	CYS
1	A	174	ASN
1	A	179	LEU
1	A	181	LEU
1	A	187	SER
1	A	205	ARG
1	A	206	GLN

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Mol	Chain	Res	Type
1	B	3	LEU
1	B	5	HIS
1	B	18	LEU
1	B	110	ASP
1	B	136	ILE
1	B	139	LEU
1	B	164	ASN
1	B	174	ASN
1	B	179	LEU
1	B	181	LEU
1	B	206	GLN
1	B	245	GLU
1	C	3	LEU
1	C	18	LEU
1	C	64	ARG
1	C	97	GLN
1	C	139	LEU
1	C	145	GLU
1	C	164	ASN
1	C	174	ASN
1	C	179	LEU
1	C	181	LEU
1	C	206	GLN
1	D	3	LEU
1	D	18	LEU
1	D	51	ILE
1	D	64	ARG
1	D	106	ARG
1	D	139	LEU
1	D	164	ASN
1	D	174	ASN
1	D	179	LEU
1	D	181	LEU
1	D	182	VAL
1	D	184	ARG
1	D	206	GLN
1	D	245	GLU
1	E	3	LEU
1	E	5	HIS
1	E	18	LEU
1	E	106	ARG
1	E	110	ASP

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Mol	Chain	Res	Type
1	E	115	ARG
1	E	123	ARG
1	E	139	LEU
1	E	145	GLU
1	E	164	ASN
1	E	174	ASN
1	E	177	ARG
1	E	179	LEU
1	E	181	LEU
1	E	206	GLN
1	F	3	LEU
1	F	5	HIS
1	F	18	LEU
1	F	123	ARG
1	F	139	LEU
1	F	160	LEU
1	F	164	ASN
1	F	174	ASN
1	F	181	LEU
1	F	205	ARG
1	F	206	GLN
1	F	226	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	HIS
1	A	28	ASN
1	A	34	GLN
1	A	36	ASN
1	A	97	GLN
1	A	103	ASN
1	A	142	GLN
1	A	164	ASN
1	A	174	ASN
1	A	206	GLN
1	A	223	HIS
1	A	240	HIS
1	A	246	GLN
1	A	252	HIS
1	B	5	HIS
1	B	28	ASN

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Mol	Chain	Res	Type
1	B	34	GLN
1	B	65	GLN
1	B	142	GLN
1	B	164	ASN
1	B	174	ASN
1	B	203	GLN
1	B	206	GLN
1	B	223	HIS
1	B	240	HIS
1	B	242	GLN
1	B	252	HIS
1	C	5	HIS
1	C	28	ASN
1	C	34	GLN
1	C	36	ASN
1	C	71	ASN
1	C	97	GLN
1	C	103	ASN
1	C	164	ASN
1	C	174	ASN
1	C	203	GLN
1	C	206	GLN
1	C	223	HIS
1	C	240	HIS
1	C	242	GLN
1	C	246	GLN
1	C	252	HIS
1	D	5	HIS
1	D	28	ASN
1	D	34	GLN
1	D	104	ASN
1	D	142	GLN
1	D	164	ASN
1	D	174	ASN
1	D	206	GLN
1	D	223	HIS
1	D	240	HIS
1	D	242	GLN
1	D	246	GLN
1	D	252	HIS
1	E	5	HIS
1	E	28	ASN

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Mol	Chain	Res	Type
1	E	34	GLN
1	E	61	GLN
1	E	97	GLN
1	E	104	ASN
1	E	142	GLN
1	E	164	ASN
1	E	174	ASN
1	E	206	GLN
1	E	223	HIS
1	E	240	HIS
1	E	242	GLN
1	E	246	GLN
1	E	252	HIS
1	F	5	HIS
1	F	28	ASN
1	F	34	GLN
1	F	104	ASN
1	F	164	ASN
1	F	174	ASN
1	F	206	GLN
1	F	240	HIS
1	F	242	GLN
1	F	246	GLN
1	F	252	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	274/274 (100%)	-0.17	3 (1%)	82 84	2, 4, 14, 19	0
1	B	271/274 (98%)	-0.24	3 (1%)	82 84	2, 5, 15, 19	0
1	C	271/274 (98%)	-0.21	6 (2%)	65 68	2, 5, 18, 24	0
1	D	271/274 (98%)	-0.29	1 (0%)	93 93	2, 5, 17, 26	0
1	E	271/274 (98%)	-0.11	4 (1%)	76 79	2, 9, 22, 27	0
1	F	274/274 (100%)	-0.25	4 (1%)	76 79	2, 6, 18, 26	0
All	All	1632/1644 (99%)	-0.21	21 (1%)	79 82	2, 6, 19, 27	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	125	GLY	2.9
1	A	226	THR	2.7
1	C	227	ASP	2.7
1	C	144	PHE	2.7
1	C	229	TYR	2.7
1	F	144	PHE	2.6
1	D	227	ASP	2.5
1	E	130	TRP	2.4
1	A	148	ASP	2.3
1	B	226	THR	2.3
1	B	229	TYR	2.3
1	A	227	ASP	2.2
1	E	145	GLU	2.2
1	E	88	LEU	2.2
1	C	226	THR	2.1
1	F	265	GLU	2.1
1	C	224	ALA	2.1
1	F	227	ASP	2.1
1	E	229	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	265	GLU	2.0
1	F	229	TYR	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, 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	LLDF	B-factors(Å^2)	Q<0.9
2	CO	E	1001	1/1	1.00	0.05	-1.76	7,7,7,7	1
2	CO	E	1002	1/1	0.98	0.04	-2.07	8,8,8,8	1
2	CO	B	1001	1/1	1.00	0.06	-2.51	4,4,4,4	1
2	CO	B	1002	1/1	0.99	0.06	-2.54	5,5,5,5	1
2	CO	F	1002	1/1	0.99	0.04	-2.90	7,7,7,7	1
2	CO	A	1001	1/1	1.00	0.05	-3.38	3,3,3,3	1
2	CO	D	1001	1/1	1.00	0.04	-3.49	4,4,4,4	1
2	CO	C	1002	1/1	0.99	0.05	-3.50	7,7,7,7	1
2	CO	F	1001	1/1	1.00	0.04	-3.57	4,4,4,4	1
2	CO	C	1001	1/1	1.00	0.05	-4.19	4,4,4,4	1
2	CO	D	1002	1/1	0.99	0.04	-4.24	6,6,6,6	1
2	CO	A	1002	1/1	0.99	0.04	-5.91	3,3,3,3	1

6.5 Other polymers (i)

There are no such residues in this entry.