



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 06:37 am BST

PDB ID : 1OHY
Title : 4-AMINO BUTYRATE-AMINOTRANSFERASE inactivated by gamma-ethynyl GABA
Authors : Storici, P.; Schirmer, T.
Deposited on : 2003-06-03
Resolution : 2.80 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

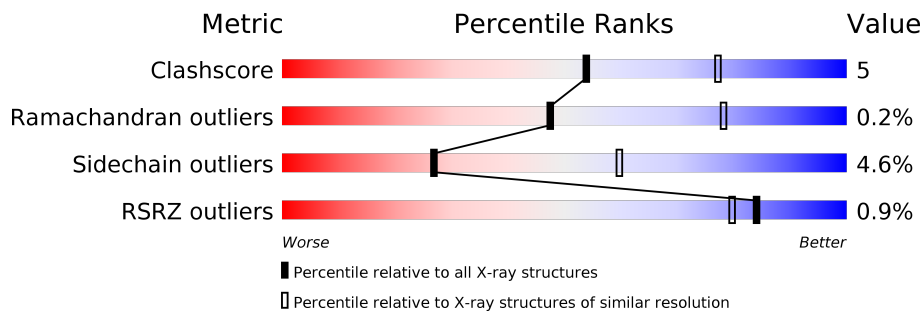
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 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 $\leq 5\%$. 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	472	 2% 81% 15% ..
1	B	472	 2% 82% 14% ..
1	C	472	 83% 14% ..
1	D	472	 82% 15% ..

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
4	FES	A	800	-	-	X	-
4	FES	C	800	-	-	X	-

2 Entry composition [i](#)

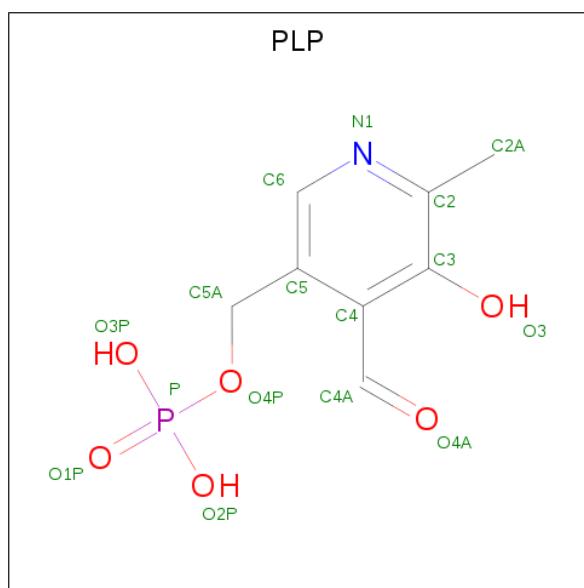
There are 5 unique types of molecules in this entry. The entry contains 14791 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 4-AMINO BUTYRATE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	461	Total 3600	C 2296	N 623	O 658	S 23	0	0	0
1	B	461	Total 3601	C 2296	N 624	O 658	S 23	0	0	0
1	C	461	Total 3601	C 2296	N 624	O 658	S 23	0	0	0
1	D	461	Total 3601	C 2296	N 624	O 658	S 23	0	0	0

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



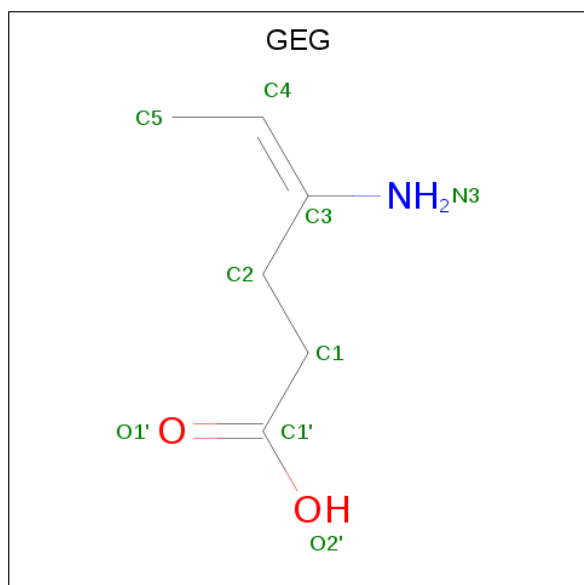
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total 15	C 8	N 1	O 5	P 1	0	0
2	B	1	Total 15	C 8	N 1	O 5	P 1	0	0

Continued on next page...

Continued from previous page...

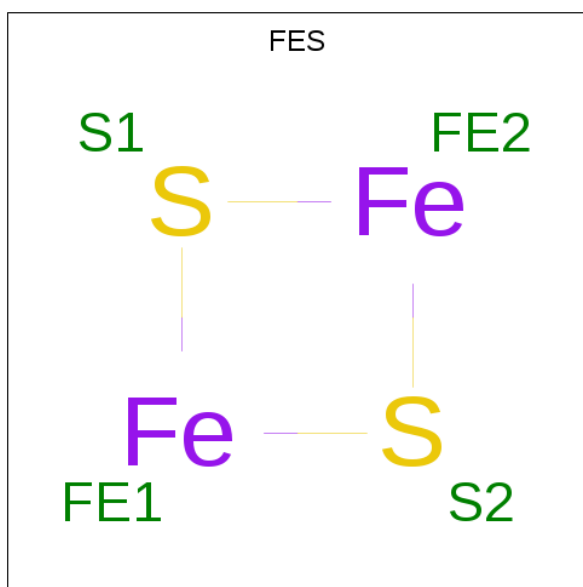
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is (4E)-4-AMINOHEX-4-ENOIC ACID (three-letter code: GEG) (formula: C₆H₁₁NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			9	6	1	2		
3	B	1	Total	C	N	O	0	0
			9	6	1	2		
3	C	1	Total	C	N	O	0	0
			9	6	1	2		
3	D	1	Total	C	N	O	0	0
			9	6	1	2		

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	C	1	Total	Fe	S	0	0
			4	2	2		

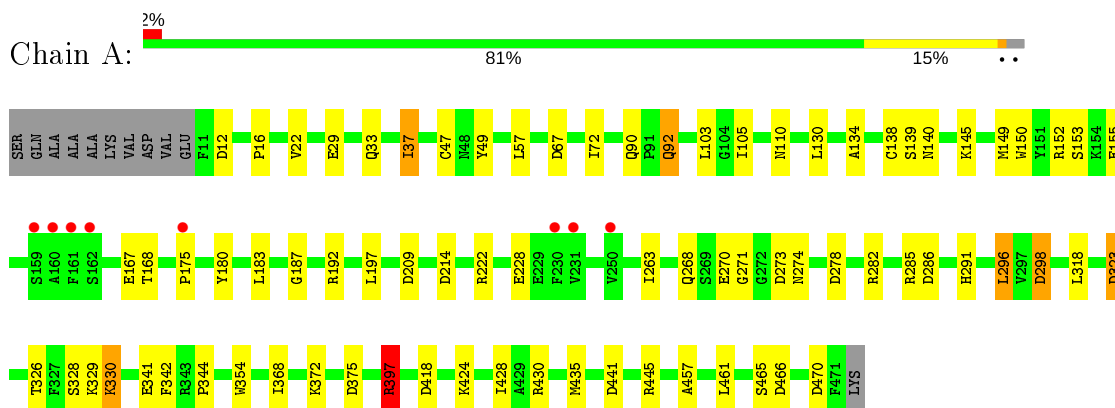
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	60	Total	O	0	0
			60	60		
5	B	55	Total	O	0	0
			55	55		
5	C	91	Total	O	0	0
			91	91		
5	D	78	Total	O	0	0
			78	78		

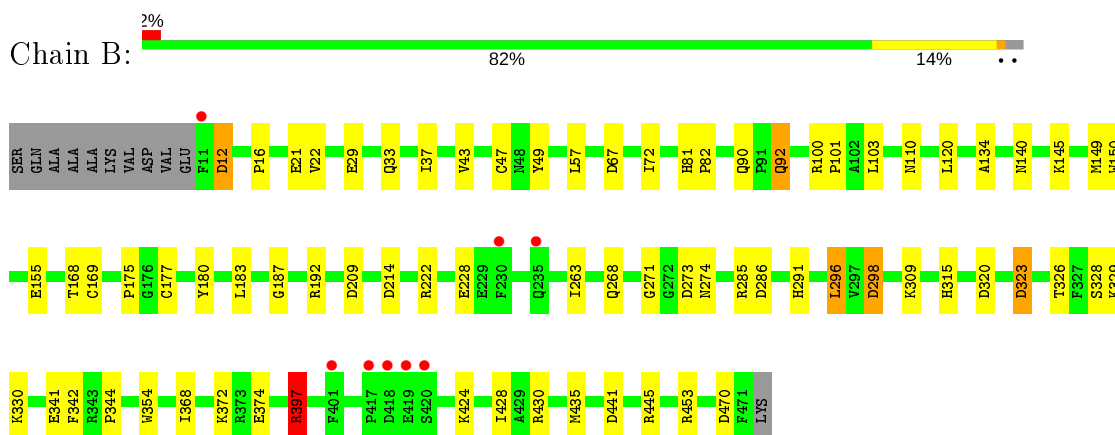
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

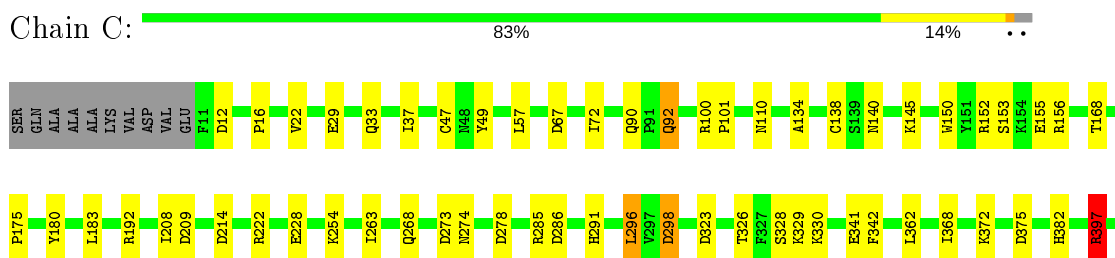
- Molecule 1: 4-AMINO BUTYRATE AMINOTRANSFERASE



- Molecule 1: 4-AMINO BUTYRATE AMINOTRANSFERASE



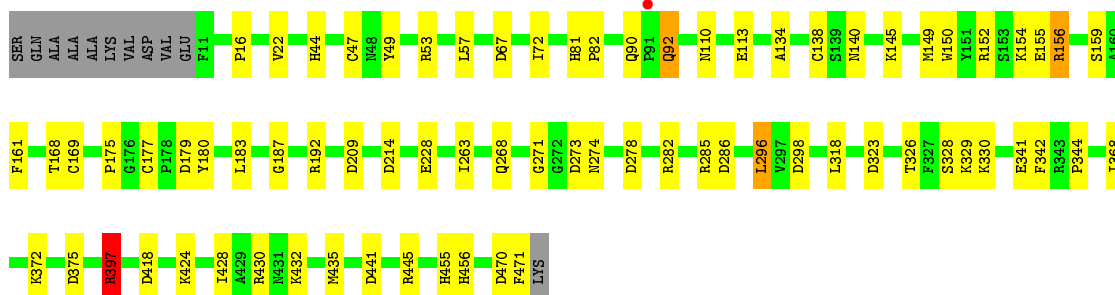
- Molecule 1: 4-AMINO BUTYRATE AMINOTRANSFERASE





- Molecule 1: 4-AMINOBTYRATE AMINOTRANSFERASE

Chain D: 82% 15% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.02Å 225.88Å 70.35Å 90.00° 108.51° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 29.42 – 2.80	Depositor EDS
% Data completeness (in resolution range)	84.8 (30.00-2.80) 84.8 (29.42-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 2.80Å)	Xtrriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.198 , 0.229 0.205 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	27.0	Xtrriage
Anisotropy	0.170	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.025 for l,-k,h	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	14791	wwPDB-VP
Average B, all atoms (Å ²)	10.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: GEG, FES, PLP

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	0.51	1/3688 (0.0%)	0.82	13/4988 (0.3%)
1	B	0.51	1/3689 (0.0%)	0.82	10/4990 (0.2%)
1	C	0.52	1/3689 (0.0%)	0.81	12/4990 (0.2%)
1	D	0.53	0/3689	0.82	10/4990 (0.2%)
All	All	0.52	3/14755 (0.0%)	0.82	45/19958 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	291	HIS	CG-ND1	6.45	1.52	1.38
1	C	291	HIS	CG-ND1	6.11	1.52	1.38
1	B	291	HIS	CG-ND1	5.18	1.50	1.38

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	286	ASP	CB-CG-OD2	6.50	124.15	118.30
1	B	286	ASP	CB-CG-OD2	6.28	123.95	118.30
1	A	466	ASP	CB-CG-OD2	6.13	123.81	118.30
1	D	286	ASP	CB-CG-OD2	6.08	123.77	118.30
1	C	298	ASP	CB-CG-OD2	6.05	123.75	118.30
1	B	298	ASP	CB-CG-OD2	6.02	123.72	118.30
1	C	67	ASP	CB-CG-OD2	6.02	123.72	118.30
1	C	214	ASP	CB-CG-OD2	5.90	123.61	118.30
1	A	286	ASP	CB-CG-OD2	5.90	123.61	118.30
1	A	470	ASP	CB-CG-OD2	5.87	123.58	118.30
1	B	12	ASP	CB-CG-OD2	5.83	123.55	118.30
1	A	298	ASP	CB-CG-OD2	5.82	123.53	118.30
1	C	12	ASP	CB-CG-OD2	5.78	123.50	118.30
1	B	67	ASP	CB-CG-OD2	5.74	123.46	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	214	ASP	CB-CG-OD2	5.71	123.44	118.30
1	D	67	ASP	CB-CG-OD2	5.65	123.38	118.30
1	A	209	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	214	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	397	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	A	375	ASP	CB-CG-OD2	5.56	123.31	118.30
1	B	397	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	A	67	ASP	CB-CG-OD2	5.55	123.29	118.30
1	C	397	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	D	397	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	D	209	ASP	CB-CG-OD2	5.45	123.20	118.30
1	D	470	ASP	CB-CG-OD2	5.44	123.20	118.30
1	C	418	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	323	ASP	CB-CG-OD2	5.30	123.07	118.30
1	C	323	ASP	CB-CG-OD2	5.29	123.06	118.30
1	D	375	ASP	CB-CG-OD2	5.28	123.05	118.30
1	B	323	ASP	CB-CG-OD2	5.27	123.05	118.30
1	C	470	ASP	CB-CG-OD2	5.26	123.03	118.30
1	B	209	ASP	CB-CG-OD2	5.23	123.01	118.30
1	C	209	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	12	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	470	ASP	CB-CG-OD2	5.19	122.97	118.30
1	B	320	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	418	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	278	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	214	ASP	CB-CG-OD2	5.12	122.91	118.30
1	D	418	ASP	CB-CG-OD2	5.12	122.91	118.30
1	D	278	ASP	CB-CG-OD2	5.11	122.90	118.30
1	C	375	ASP	CB-CG-OD2	5.06	122.85	118.30
1	D	298	ASP	CB-CG-OD2	5.04	122.83	118.30
1	C	278	ASP	CB-CG-OD2	5.02	122.82	118.30

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	3600	0	3501	45	1
1	B	3601	0	3503	42	0
1	C	3601	0	3503	35	1
1	D	3601	0	3503	41	1
2	A	15	0	7	2	0
2	B	15	0	7	2	0
2	C	15	0	7	2	0
2	D	15	0	7	1	0
3	A	9	0	7	4	0
3	B	9	0	7	4	0
3	C	9	0	7	4	0
3	D	9	0	7	4	0
4	A	4	0	0	4	0
4	C	4	0	0	4	0
5	A	60	0	0	2	0
5	B	55	0	0	3	0
5	C	91	0	0	1	0
5	D	78	0	0	4	0
All	All	14791	0	14066	152	2

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 (152) 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:B:374:GLU:HG3	5:B:2046:HOH:O	1.65	0.95
1:C:72:ILE:CG2	3:C:700:GEG:H5C2	2.12	0.79
1:B:72:ILE:CG2	3:B:700:GEG:H5C2	2.12	0.79
1:A:138:CYS:HB3	4:A:800:FES:S2	2.23	0.77
1:A:72:ILE:CG2	3:A:700:GEG:H5C2	2.14	0.77
1:D:72:ILE:CG2	3:D:700:GEG:H5C2	2.17	0.75
1:C:397:ARG:HH11	1:C:397:ARG:HG2	1.54	0.73
1:A:397:ARG:HH11	1:A:397:ARG:HG2	1.54	0.72
1:D:397:ARG:HH11	1:D:397:ARG:HG2	1.54	0.71
1:B:397:ARG:HG2	1:B:397:ARG:HH11	1.54	0.70
1:C:152:ARG:HD2	1:C:180:TYR:HE1	1.57	0.69
1:C:152:ARG:HD2	1:C:180:TYR:CE1	2.27	0.69
1:C:329:LYS:NZ	2:C:600:PLP:C4A	2.57	0.66
1:A:152:ARG:HD2	1:A:180:TYR:HE1	1.60	0.66
1:B:397:ARG:CG	1:B:397:ARG:HH11	2.12	0.63
1:C:397:ARG:HH11	1:C:397:ARG:CG	2.11	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:179:ASP:HB2	5:D:2028:HOH:O	1.98	0.63
1:D:397:ARG:HH11	1:D:397:ARG:CG	2.11	0.62
1:A:397:ARG:HH11	1:A:397:ARG:CG	2.12	0.61
1:B:309:LYS:HG3	1:B:315:HIS:CE1	2.35	0.61
1:C:382:HIS:NE2	1:C:454:ASP:OD2	2.33	0.61
1:A:134:ALA:HB3	4:A:800:FES:S1	2.41	0.60
1:A:22:VAL:HG11	1:A:430:ARG:HD3	1.84	0.60
1:A:72:ILE:HG21	3:A:700:GEG:H5C2	1.84	0.59
1:B:22:VAL:HG11	1:B:430:ARG:HD3	1.84	0.59
1:A:152:ARG:HD2	1:A:180:TYR:CE1	2.38	0.58
1:C:155:GLU:OE1	1:C:180:TYR:OH	2.19	0.58
1:C:22:VAL:HG11	1:C:430:ARG:HD3	1.84	0.58
1:D:22:VAL:HG11	1:D:430:ARG:HD3	1.84	0.58
1:C:72:ILE:HG21	3:C:700:GEG:H5C2	1.82	0.57
1:C:138:CYS:HB3	4:C:800:FES:S2	2.45	0.56
1:B:155:GLU:OE1	1:B:180:TYR:OH	2.23	0.56
1:A:155:GLU:OE1	1:A:180:TYR:OH	2.19	0.56
1:A:329:LYS:NZ	2:A:600:PLP:C4A	2.65	0.56
1:B:329:LYS:NZ	2:B:600:PLP:C4A	2.70	0.55
1:B:72:ILE:HG22	3:B:700:GEG:H5C2	1.88	0.55
4:C:800:FES:S2	1:D:138:CYS:HB3	2.47	0.55
1:D:471:PHE:C	5:D:2077:HOH:O	2.45	0.54
1:A:268:GLN:O	1:A:273:ASP:HA	2.08	0.54
1:C:192:ARG:HB3	1:D:145:LYS:HZ3	1.73	0.54
1:B:72:ILE:HG21	3:B:700:GEG:H5C2	1.89	0.54
1:C:268:GLN:O	1:C:273:ASP:HA	2.08	0.54
1:D:90:GLN:HB3	1:D:92:GLN:NE2	2.24	0.53
1:B:268:GLN:O	1:B:273:ASP:HA	2.09	0.53
1:D:329:LYS:NZ	2:D:600:PLP:C4A	2.71	0.53
1:D:268:GLN:O	1:D:273:ASP:HA	2.08	0.52
1:A:90:GLN:HB3	1:A:92:GLN:NE2	2.25	0.52
1:A:192:ARG:HB3	1:B:145:LYS:NZ	2.26	0.51
1:B:90:GLN:HB3	1:B:92:GLN:NE2	2.25	0.51
1:D:72:ILE:HG21	3:D:700:GEG:H5C2	1.90	0.51
1:C:192:ARG:HB3	1:D:145:LYS:NZ	2.25	0.51
1:C:90:GLN:HB3	1:C:92:GLN:NE2	2.26	0.50
1:A:192:ARG:HB3	1:B:145:LYS:HZ3	1.77	0.50
1:A:145:LYS:HZ3	1:B:192:ARG:HB3	1.76	0.50
1:D:155:GLU:OE1	1:D:180:TYR:OH	2.30	0.50
1:D:22:VAL:CG1	1:D:430:ARG:HD3	2.43	0.49
1:A:150:TRP:CD2	1:A:342:PHE:CE2	3.01	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:TRP:CD2	1:C:342:PHE:CE2	3.01	0.49
1:C:22:VAL:CG1	1:C:430:ARG:HD3	2.43	0.49
1:D:150:TRP:CD2	1:D:342:PHE:CE2	3.00	0.49
1:A:22:VAL:CG1	1:A:430:ARG:HD3	2.43	0.49
1:B:150:TRP:CD2	1:B:342:PHE:CE2	3.01	0.49
1:B:22:VAL:CG1	1:B:430:ARG:HD3	2.43	0.48
1:A:138:CYS:CB	4:A:800:FES:S2	2.93	0.48
1:A:298:ASP:OD1	2:A:600:PLP:N1	2.46	0.48
1:A:72:ILE:HB	3:A:700:GEG:C5	2.44	0.47
1:D:168:THR:HG21	1:D:175:PRO:HD2	1.96	0.47
1:A:168:THR:HG21	1:A:175:PRO:HD2	1.96	0.47
1:C:47:CYS:HB2	1:C:49:TYR:CE2	2.49	0.47
1:A:47:CYS:HB2	1:A:49:TYR:CE2	2.49	0.47
1:C:168:THR:HG21	1:C:175:PRO:HD2	1.96	0.47
1:C:57:LEU:HD23	1:C:435:MET:SD	2.54	0.47
1:D:81:HIS:ND1	1:D:82:PRO:HD2	2.30	0.47
1:C:298:ASP:OD1	2:C:600:PLP:N1	2.47	0.46
1:C:183:LEU:HD23	1:C:183:LEU:C	2.36	0.46
1:A:183:LEU:C	1:A:183:LEU:HD23	2.35	0.46
1:B:168:THR:HG21	1:B:175:PRO:HD2	1.96	0.46
1:D:183:LEU:HD23	1:D:183:LEU:C	2.36	0.46
1:A:37:ILE:HG21	1:B:120:LEU:HD21	1.97	0.46
1:B:57:LEU:HD23	1:B:435:MET:SD	2.56	0.46
1:C:362:LEU:O	5:C:2073:HOH:O	2.21	0.46
1:B:47:CYS:HB2	1:B:49:TYR:CE2	2.50	0.46
4:C:800:FES:S1	1:D:134:ALA:HB3	2.56	0.46
1:D:47:CYS:HB2	1:D:49:TYR:CE2	2.51	0.46
1:B:183:LEU:HD23	1:B:183:LEU:C	2.36	0.45
1:D:152:ARG:HD2	1:D:180:TYR:CE1	2.51	0.45
1:D:155:GLU:OE2	1:D:180:TYR:OH	2.35	0.45
1:B:263:ILE:HA	1:B:296:LEU:O	2.17	0.45
1:C:263:ILE:HA	1:C:296:LEU:O	2.17	0.45
1:A:330:LYS:HD3	5:A:2035:HOH:O	2.17	0.45
1:B:100:ARG:HA	1:B:101:PRO:HD3	1.81	0.45
1:C:268:GLN:HB2	1:C:274:ASN:HB2	1.98	0.44
1:D:263:ILE:HA	1:D:296:LEU:O	2.17	0.44
1:A:268:GLN:HB2	1:A:274:ASN:HB2	1.99	0.44
1:A:57:LEU:HD23	1:A:435:MET:SD	2.57	0.44
1:A:270:GLU:HG2	5:A:2059:HOH:O	2.17	0.44
1:B:424:LYS:O	1:B:428:ILE:HG12	2.18	0.44
1:A:263:ILE:HA	1:A:296:LEU:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:ILE:HB	3:C:700:GEG:C5	2.47	0.44
1:A:397:ARG:NH1	1:A:397:ARG:CG	2.79	0.44
1:B:374:GLU:CG	5:B:2046:HOH:O	2.44	0.44
1:A:457:ALA:O	1:A:461:LEU:HG	2.17	0.44
1:B:140:ASN:OD1	1:B:326:THR:HG21	2.18	0.44
1:B:81:HIS:HA	1:B:82:PRO:HD3	1.87	0.44
1:B:268:GLN:HB2	1:B:274:ASN:HB2	1.99	0.43
1:C:145:LYS:NZ	1:D:192:ARG:HB3	2.33	0.43
1:D:57:LEU:HD23	1:D:435:MET:SD	2.58	0.43
1:A:145:LYS:NZ	1:B:192:ARG:HB3	2.33	0.43
1:A:105:ILE:HA	1:B:43:VAL:HA	1.99	0.43
1:C:424:LYS:O	1:C:428:ILE:HG12	2.18	0.43
1:A:72:ILE:CB	3:A:700:GEG:H5C2	2.49	0.43
1:D:179:ASP:CB	5:D:2028:HOH:O	2.62	0.43
1:B:29:GLU:OE2	1:B:33:GLN:NE2	2.50	0.43
1:C:208:ILE:HD13	1:D:161:PHE:CD2	2.53	0.43
1:A:424:LYS:O	1:A:428:ILE:HG12	2.18	0.43
1:B:145:LYS:NZ	5:B:2017:HOH:O	2.50	0.43
1:D:268:GLN:HB2	1:D:274:ASN:HB2	1.99	0.43
1:D:113:GLU:CB	5:D:2016:HOH:O	2.65	0.43
1:C:100:ARG:HA	1:C:101:PRO:HD3	1.80	0.43
1:C:140:ASN:OD1	1:C:326:THR:HG21	2.18	0.43
1:B:298:ASP:OD1	2:B:600:PLP:N1	2.52	0.42
1:D:72:ILE:HG22	3:D:700:GEG:H5C2	1.98	0.42
1:B:169:CYS:HA	1:B:177:CYS:SG	2.59	0.42
1:C:153:SER:HA	1:C:156:ARG:HG2	2.01	0.42
1:D:140:ASN:OD1	1:D:326:THR:HG21	2.19	0.42
1:D:424:LYS:O	1:D:428:ILE:HG12	2.19	0.42
1:D:149:MET:HE1	1:D:344:PRO:HB3	2.02	0.42
4:A:800:FES:S1	1:B:134:ALA:HB3	2.60	0.42
1:C:134:ALA:HB3	4:C:800:FES:S1	2.60	0.42
1:A:29:GLU:OE2	1:A:33:GLN:NE2	2.51	0.42
1:D:187:GLY:O	1:D:271:GLY:HA3	2.20	0.42
1:D:72:ILE:HB	3:D:700:GEG:C5	2.50	0.41
1:B:72:ILE:HB	3:B:700:GEG:C5	2.50	0.41
1:A:140:ASN:OD1	1:A:326:THR:HG21	2.21	0.41
1:A:323:ASP:HB3	1:A:342:PHE:CE1	2.56	0.41
1:B:187:GLY:O	1:B:271:GLY:HA3	2.21	0.41
1:C:29:GLU:OE2	1:C:33:GLN:NE2	2.50	0.41
1:D:169:CYS:HA	1:D:177:CYS:SG	2.61	0.41
1:D:397:ARG:NH1	1:D:397:ARG:HG2	2.30	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:323:ASP:HB3	1:D:342:PHE:CE1	2.56	0.41
1:A:130:LEU:HB3	1:B:37:ILE:HG23	2.03	0.41
1:D:455:HIS:NE2	1:D:456:HIS:CE1	2.89	0.41
1:A:282:ARG:CD	1:A:318:LEU:HD21	2.51	0.40
1:A:149:MET:HE1	1:A:344:PRO:HB3	2.03	0.40
1:A:197:LEU:HD12	1:A:197:LEU:HA	1.94	0.40
1:A:187:GLY:O	1:A:271:GLY:HA3	2.21	0.40
1:A:103:LEU:HD12	1:A:354:TRP:O	2.22	0.40
1:B:323:ASP:HB3	1:B:342:PHE:CE1	2.55	0.40
1:D:282:ARG:CD	1:D:318:LEU:HD21	2.51	0.40
1:B:103:LEU:HD12	1:B:354:TRP:O	2.21	0.40
1:B:149:MET:HE1	1:B:344:PRO:HB3	2.02	0.40
1:C:72:ILE:CB	3:C:700:GEG:H5C2	2.51	0.40

All (2) 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:D:156:ARG:O	1:D:432:LYS:NZ[1_455]	2.02	0.18
1:A:167:GLU:OE2	1:C:254:LYS:CE[2_647]	2.06	0.14

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	459/472 (97%)	434 (95%)	24 (5%)	1 (0%)	47 78
1	B	459/472 (97%)	436 (95%)	22 (5%)	1 (0%)	47 78
1	C	459/472 (97%)	432 (94%)	26 (6%)	1 (0%)	47 78
1	D	459/472 (97%)	436 (95%)	22 (5%)	1 (0%)	47 78
All	All	1836/1888 (97%)	1738 (95%)	94 (5%)	4 (0%)	47 78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	SER
1	B	328	SER
1	C	328	SER
1	D	328	SER

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	383/408 (94%)	365 (95%)	18 (5%)	26	59
1	B	383/408 (94%)	366 (96%)	17 (4%)	28	61
1	C	383/408 (94%)	366 (96%)	17 (4%)	28	61
1	D	383/408 (94%)	365 (95%)	18 (5%)	26	59
All	All	1532/1632 (94%)	1462 (95%)	70 (5%)	27	60

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	PRO
1	A	37	ILE
1	A	92	GLN
1	A	110	ASN
1	A	139	SER
1	A	153	SER
1	A	222	ARG
1	A	228	GLU
1	A	285	ARG
1	A	296	LEU
1	A	330	LYS
1	A	341	GLU
1	A	368	ILE
1	A	372	LYS
1	A	397	ARG
1	A	441	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	445	ARG
1	A	465	SER
1	B	12	ASP
1	B	16	PRO
1	B	21	GLU
1	B	92	GLN
1	B	110	ASN
1	B	222	ARG
1	B	228	GLU
1	B	285	ARG
1	B	296	LEU
1	B	330	LYS
1	B	341	GLU
1	B	368	ILE
1	B	372	LYS
1	B	397	ARG
1	B	441	ASP
1	B	445	ARG
1	B	453	ARG
1	C	16	PRO
1	C	37	ILE
1	C	92	GLN
1	C	110	ASN
1	C	222	ARG
1	C	228	GLU
1	C	285	ARG
1	C	296	LEU
1	C	330	LYS
1	C	341	GLU
1	C	368	ILE
1	C	372	LYS
1	C	397	ARG
1	C	441	ASP
1	C	445	ARG
1	C	465	SER
1	C	470	ASP
1	D	16	PRO
1	D	44	HIS
1	D	53	ARG
1	D	92	GLN
1	D	110	ASN
1	D	154	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	156	ARG
1	D	159	SER
1	D	228	GLU
1	D	285	ARG
1	D	296	LEU
1	D	330	LYS
1	D	341	GLU
1	D	368	ILE
1	D	372	LYS
1	D	397	ARG
1	D	441	ASP
1	D	445	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	92	GLN
1	A	110	ASN
1	B	55	ASN
1	B	92	GLN
1	B	110	ASN
1	B	275	HIS
1	C	55	ASN
1	C	92	GLN
1	C	110	ASN
1	D	92	GLN
1	D	110	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

10 ligands are modelled in this entry.

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
2	PLP	C	600	3	15,15,16	1.03	1 (6%)	20,22,23	1.59	3 (15%)
2	PLP	A	600	3	15,15,16	1.08	1 (6%)	20,22,23	1.03	2 (10%)
2	PLP	D	600	3	15,15,16	1.06	2 (13%)	20,22,23	1.13	2 (10%)
2	PLP	B	600	3	15,15,16	0.95	1 (6%)	20,22,23	1.36	3 (15%)
4	FES	A	800	1	0,4,4	0.00	-	-	-	-
3	GEG	B	700	1,2	5,8,8	3.18	2 (40%)	4,9,9	2.70	1 (25%)
3	GEG	D	700	1,2	5,8,8	2.73	2 (40%)	4,9,9	3.59	1 (25%)
4	FES	C	800	1	0,4,4	0.00	-	-	-	-
3	GEG	A	700	1,2	5,8,8	3.02	2 (40%)	4,9,9	3.75	1 (25%)
3	GEG	C	700	1,2	5,8,8	2.75	2 (40%)	4,9,9	3.33	1 (25%)

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
2	PLP	C	600	3	-	0/6/6/8	0/1/1/1
2	PLP	A	600	3	-	0/6/6/8	0/1/1/1
2	PLP	D	600	3	-	0/6/6/8	0/1/1/1
2	PLP	B	600	3	-	0/6/6/8	0/1/1/1
4	FES	A	800	1	-	-	0/1/1/1
3	GEG	B	700	1,2	-	3/4/7/7	-
3	GEG	D	700	1,2	-	3/4/7/7	-
4	FES	C	800	1	-	-	0/1/1/1
3	GEG	A	700	1,2	-	3/4/7/7	-
3	GEG	C	700	1,2	-	2/4/7/7	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	700	GEG	C3-N3	5.75	1.46	1.33
3	A	700	GEG	C3-N3	5.50	1.46	1.33
3	C	700	GEG	C3-N3	5.26	1.45	1.33
3	D	700	GEG	C3-N3	4.94	1.44	1.33
3	B	700	GEG	C2-C3	4.17	1.54	1.50
3	A	700	GEG	C2-C3	3.67	1.54	1.50
3	D	700	GEG	C2-C3	3.53	1.53	1.50
3	C	700	GEG	C2-C3	3.13	1.53	1.50
2	D	600	PLP	C2-N1	2.39	1.38	1.33
2	A	600	PLP	C2-N1	2.24	1.38	1.33
2	C	600	PLP	C2-N1	2.17	1.38	1.33
2	B	600	PLP	C2-N1	2.13	1.37	1.33
2	D	600	PLP	C6-N1	2.12	1.38	1.34

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	700	GEG	C4-C3-N3	-7.47	114.70	123.28
3	D	700	GEG	C4-C3-N3	-7.05	115.18	123.28
3	C	700	GEG	C4-C3-N3	-6.57	115.74	123.28
3	B	700	GEG	C4-C3-N3	-5.33	117.16	123.28
2	C	600	PLP	C4A-C4-C5	-4.78	116.01	120.94
2	B	600	PLP	C4A-C4-C5	-3.86	116.96	120.94
2	D	600	PLP	C4A-C4-C5	-2.90	117.95	120.94
2	C	600	PLP	C5-C6-N1	-2.67	119.38	123.82
2	B	600	PLP	C5-C6-N1	-2.36	119.89	123.82
2	D	600	PLP	C5-C6-N1	-2.27	120.04	123.82
2	C	600	PLP	C3-C4-C5	2.22	121.14	118.74
2	A	600	PLP	C5-C6-N1	-2.10	120.33	123.82
2	A	600	PLP	C4A-C4-C5	-2.08	118.80	120.94
2	B	600	PLP	C3-C4-C5	2.07	120.98	118.74

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	700	GEG	C1-C2-C3-C4
3	D	700	GEG	C1'-C1-C2-C3
3	D	700	GEG	C1-C2-C3-C4
3	A	700	GEG	C1'-C1-C2-C3
3	A	700	GEG	C1-C2-C3-C4
3	C	700	GEG	C1'-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	700	GEG	C1'-C1-C2-C3
3	C	700	GEG	C1-C2-C3-N3
3	A	700	GEG	C1-C2-C3-N3
3	B	700	GEG	C1-C2-C3-N3
3	D	700	GEG	C1-C2-C3-N3

There are no ring outliers.

10 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	600	PLP	2	0
2	A	600	PLP	2	0
2	D	600	PLP	1	0
2	B	600	PLP	2	0
4	A	800	FES	4	0
3	B	700	GEG	4	0
3	D	700	GEG	4	0
4	C	800	FES	4	0
3	A	700	GEG	4	0
3	C	700	GEG	4	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	461/472 (97%)	-0.24	8 (1%) 70 63	10, 11, 11, 11	0
1	B	461/472 (97%)	-0.08	8 (1%) 70 63	10, 11, 11, 11	0
1	C	461/472 (97%)	-0.41	0 100 100	10, 11, 11, 11	0
1	D	461/472 (97%)	-0.53	1 (0%) 95 94	10, 11, 11, 12	0
All	All	1844/1888 (97%)	-0.32	17 (0%) 84 80	10, 11, 11, 12	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	420	SER	3.1
1	B	418	ASP	3.1
1	D	91	PRO	2.9
1	A	162	SER	2.9
1	B	419	GLU	2.8
1	A	161	PHE	2.8
1	A	230	PHE	2.7
1	B	11	PHE	2.5
1	B	230	PHE	2.5
1	B	235	GLN	2.5
1	A	231	VAL	2.4
1	A	159	SER	2.3
1	A	160	ALA	2.3
1	A	175	PRO	2.2
1	B	417	PRO	2.1
1	A	250	VAL	2.1
1	B	401	PHE	2.1

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

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

6.3 Carbohydrates [i](#)

There are no 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. 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	B-factors(Å ²)	Q<0.9
3	GEG	D	700	9/9	0.93	0.15	11,11,11,11	0
3	GEG	A	700	9/9	0.96	0.17	11,11,11,11	0
3	GEG	C	700	9/9	0.96	0.14	11,11,11,11	0
3	GEG	B	700	9/9	0.97	0.16	11,11,12,12	0
2	PLP	A	600	15/16	0.98	0.12	10,11,11,11	0
2	PLP	D	600	15/16	0.98	0.11	10,11,11,11	0
4	FES	C	800	4/4	0.98	0.20	13,13,13,15	0
2	PLP	B	600	15/16	0.98	0.13	10,11,11,11	0
4	FES	A	800	4/4	0.98	0.22	13,14,14,15	0
2	PLP	C	600	15/16	0.99	0.08	10,11,11,11	0

6.5 Other polymers [i](#)

There are no such residues in this entry.