



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:10 PM GMT

PDB ID : 4GRX
Title : Structure of an omega-aminotransferase from *Paracoccus denitrificans*
Authors : Rausch, C.; Lerchner, A.; Schiefner, A.; Skerra, A.
Deposited on : 2012-08-27
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

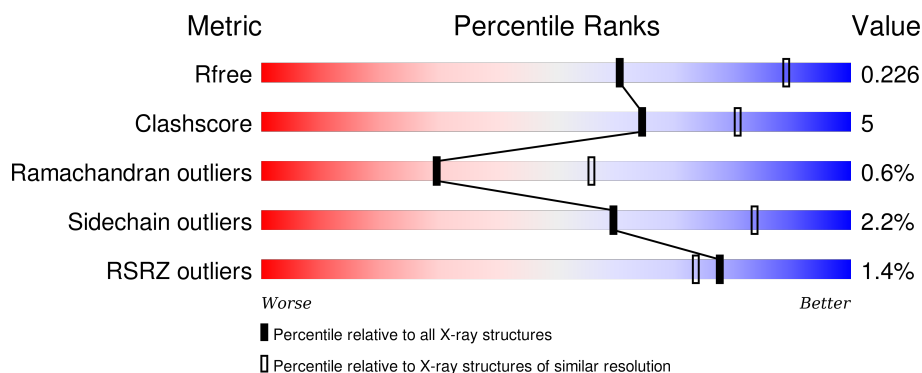
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	465	 85% 11% • •
1	B	465	 86% 11% •
1	C	465	 82% 14% • •
1	D	465	 83% 13% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DAV	A	502	-	-	-	X
3	DAV	C	502	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14277 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 Aminotransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	449	Total	C	N	O	P	S	0	0	0
			3503	2241	594	645	1	22			
1	B	449	Total	C	N	O	P	S	0	0	0
			3503	2241	594	645	1	22			
1	C	449	Total	C	N	O	P	S	0	0	0
			3503	2241	594	645	1	22			
1	D	449	Total	C	N	O	P	S	0	0	0
			3503	2241	594	645	1	22			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	EXPRESSION TAG	UNP A1B956
A	-10	ALA	-	EXPRESSION TAG	UNP A1B956
A	-9	SER	-	EXPRESSION TAG	UNP A1B956
A	-8	TRP	-	EXPRESSION TAG	UNP A1B956
A	-7	SER	-	EXPRESSION TAG	UNP A1B956
A	-6	HIS	-	EXPRESSION TAG	UNP A1B956
A	-5	PRO	-	EXPRESSION TAG	UNP A1B956
A	-4	GLN	-	EXPRESSION TAG	UNP A1B956
A	-3	PHE	-	EXPRESSION TAG	UNP A1B956
A	-2	GLU	-	EXPRESSION TAG	UNP A1B956
A	-1	LYS	-	EXPRESSION TAG	UNP A1B956
A	0	GLY	-	EXPRESSION TAG	UNP A1B956
A	1	ALA	-	EXPRESSION TAG	UNP A1B956
B	-11	MET	-	EXPRESSION TAG	UNP A1B956
B	-10	ALA	-	EXPRESSION TAG	UNP A1B956
B	-9	SER	-	EXPRESSION TAG	UNP A1B956
B	-8	TRP	-	EXPRESSION TAG	UNP A1B956
B	-7	SER	-	EXPRESSION TAG	UNP A1B956
B	-6	HIS	-	EXPRESSION TAG	UNP A1B956
B	-5	PRO	-	EXPRESSION TAG	UNP A1B956
B	-4	GLN	-	EXPRESSION TAG	UNP A1B956

Continued on next page...

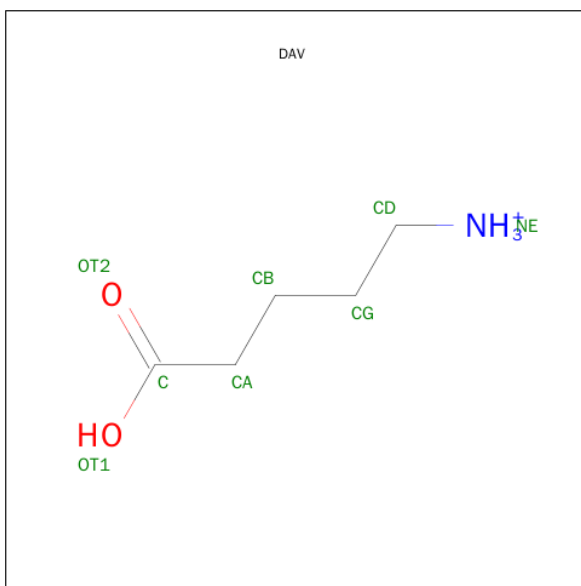
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	PHE	-	EXPRESSION TAG	UNP A1B956
B	-2	GLU	-	EXPRESSION TAG	UNP A1B956
B	-1	LYS	-	EXPRESSION TAG	UNP A1B956
B	0	GLY	-	EXPRESSION TAG	UNP A1B956
B	1	ALA	-	EXPRESSION TAG	UNP A1B956
C	-11	MET	-	EXPRESSION TAG	UNP A1B956
C	-10	ALA	-	EXPRESSION TAG	UNP A1B956
C	-9	SER	-	EXPRESSION TAG	UNP A1B956
C	-8	TRP	-	EXPRESSION TAG	UNP A1B956
C	-7	SER	-	EXPRESSION TAG	UNP A1B956
C	-6	HIS	-	EXPRESSION TAG	UNP A1B956
C	-5	PRO	-	EXPRESSION TAG	UNP A1B956
C	-4	GLN	-	EXPRESSION TAG	UNP A1B956
C	-3	PHE	-	EXPRESSION TAG	UNP A1B956
C	-2	GLU	-	EXPRESSION TAG	UNP A1B956
C	-1	LYS	-	EXPRESSION TAG	UNP A1B956
C	0	GLY	-	EXPRESSION TAG	UNP A1B956
C	1	ALA	-	EXPRESSION TAG	UNP A1B956
D	-11	MET	-	EXPRESSION TAG	UNP A1B956
D	-10	ALA	-	EXPRESSION TAG	UNP A1B956
D	-9	SER	-	EXPRESSION TAG	UNP A1B956
D	-8	TRP	-	EXPRESSION TAG	UNP A1B956
D	-7	SER	-	EXPRESSION TAG	UNP A1B956
D	-6	HIS	-	EXPRESSION TAG	UNP A1B956
D	-5	PRO	-	EXPRESSION TAG	UNP A1B956
D	-4	GLN	-	EXPRESSION TAG	UNP A1B956
D	-3	PHE	-	EXPRESSION TAG	UNP A1B956
D	-2	GLU	-	EXPRESSION TAG	UNP A1B956
D	-1	LYS	-	EXPRESSION TAG	UNP A1B956
D	0	GLY	-	EXPRESSION TAG	UNP A1B956
D	1	ALA	-	EXPRESSION TAG	UNP A1B956

- 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

- Molecule 3 is DELTA-AMINO VALERIC ACID (three-letter code: DAV) (formula: $C_5H_{12}NO_2$).



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

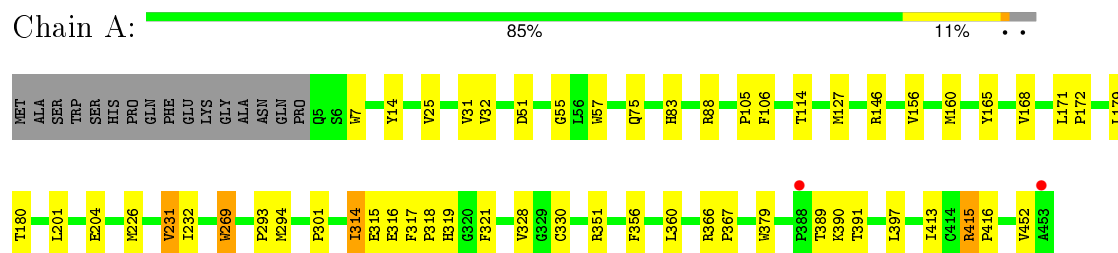
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	74	Total	O	0	0
			74	74		
4	B	59	Total	O	0	0
			59	59		
4	C	64	Total	O	0	0
			64	64		
4	D	48	Total	O	0	0
			48	48		

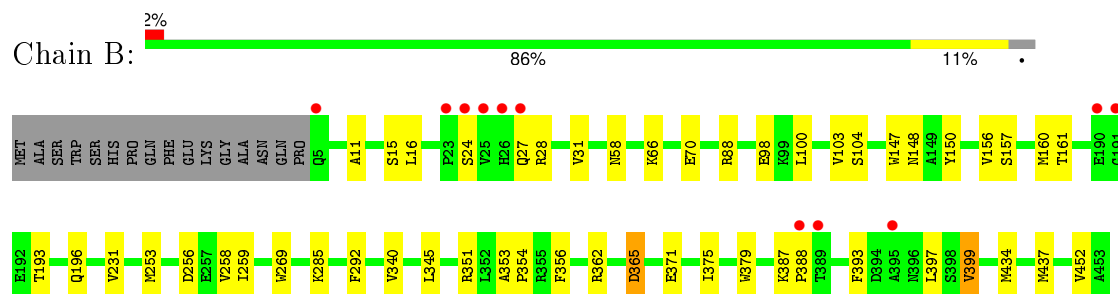
3 Residue-property plots [i](#)

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.

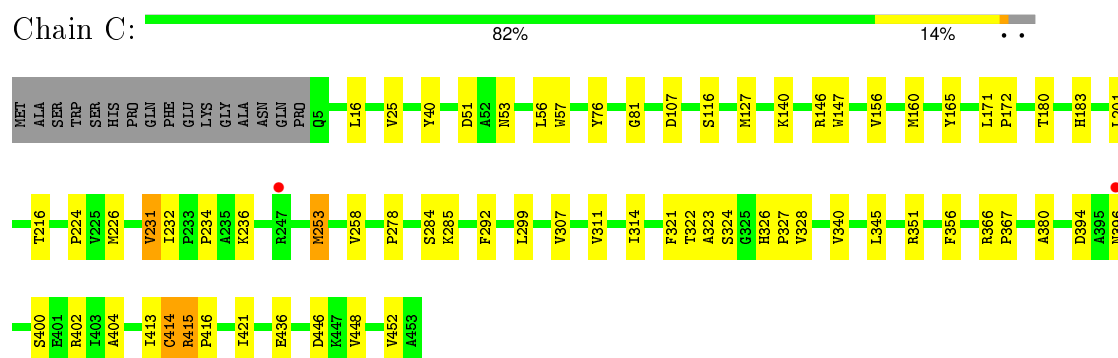
• Molecule 1: Aminotransferase



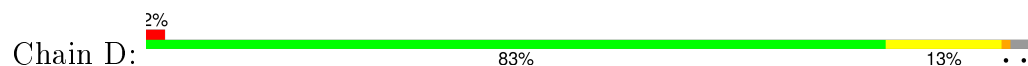
• Molecule 1: Aminotransferase

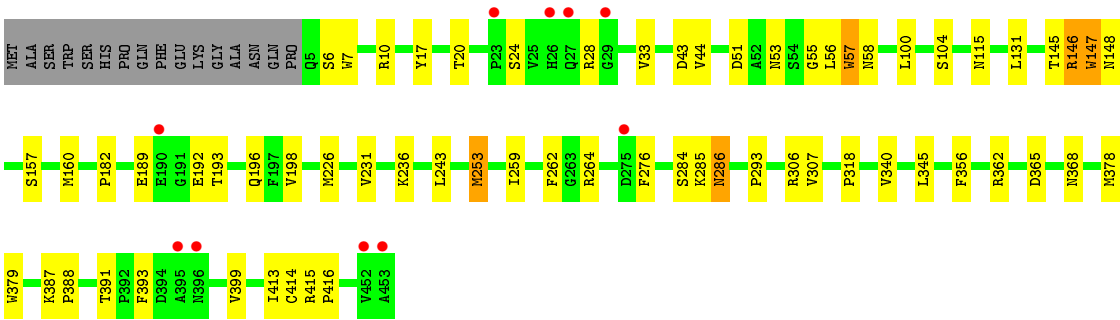


• Molecule 1: Aminotransferase



• Molecule 1: Aminotransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.79Å 103.63Å 145.43Å 90.00° 98.88° 90.00°	Depositor
Resolution (Å)	19.83 – 2.60 19.83 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.83-2.60) 99.8 (19.83-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.178 , 0.227 0.177 , 0.226	Depositor DCC
R_{free} test set	3063 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	35.9	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 32.3	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 60090 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14277	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NA, DAV, LLP

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	0.56	2/3569 (0.1%)	0.63	0/4839
1	B	0.55	2/3569 (0.1%)	0.64	0/4839
1	C	0.55	1/3569 (0.0%)	0.63	0/4839
1	D	0.53	3/3569 (0.1%)	0.60	0/4839
All	All	0.55	8/14276 (0.1%)	0.62	0/19356

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	147	TRP	CD2-CE2	5.53	1.48	1.41
1	C	147	TRP	CD2-CE2	5.53	1.48	1.41
1	A	269	TRP	CD2-CE2	5.17	1.47	1.41
1	B	379	TRP	CD2-CE2	5.16	1.47	1.41
1	B	269	TRP	CD2-CE2	5.14	1.47	1.41
1	D	379	TRP	CD2-CE2	5.05	1.47	1.41
1	A	57	TRP	CD2-CE2	5.04	1.47	1.41
1	D	57	TRP	CD2-CE2	5.04	1.47	1.41

There are no bond angle outliers.

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	3503	0	3423	37	0
1	B	3503	0	3423	34	0
1	C	3503	0	3423	41	0
1	D	3503	0	3423	39	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
3	A	8	0	11	0	0
3	C	8	0	11	2	0
4	A	74	0	0	1	0
4	B	59	0	0	0	0
4	C	64	0	0	1	0
4	D	48	0	0	2	0
All	All	14277	0	13714	140	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 (140) 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:157:SER:HA	1:D:160:MET:HE2	1.57	0.87
1:D:253:MET:HE2	1:D:276:PHE:HE2	1.45	0.81
1:B:147:TRP:O	1:B:148:ASN:HB2	1.77	0.81
1:C:400:SER:HB2	1:C:416:PRO:HB2	1.67	0.76
1:D:253:MET:HE2	1:D:276:PHE:CE2	2.23	0.74
1:B:256:ASP:OD1	1:B:285:LLP:H2'2	1.89	0.73
1:D:157:SER:HA	1:D:160:MET:CE	2.16	0.73
1:A:51:ASP:HA	1:A:413:ILE:HB	1.71	0.72
1:D:7:TRP:CD1	1:D:44:VAL:HG21	2.25	0.72
1:B:193:THR:HG22	1:B:196:GLN:HG3	1.72	0.72
1:C:285:LLP:H4'1	3:C:502:DAV:NE	2.10	0.67
1:A:127:MET:HE2	1:B:16:LEU:HD21	1.78	0.66
1:B:362:ARG:O	1:B:365:ASP:HB2	1.97	0.64
1:B:58:ASN:HB3	1:B:285:LLP:HG3	1.79	0.64
1:D:286:ASN:HB2	4:D:610:HOH:O	1.98	0.63
1:D:17:TYR:HB3	1:D:20:THR:HB	1.80	0.63
1:A:452:VAL:O	1:A:452:VAL:HG12	2.00	0.62
1:C:415:ARG:NH1	1:C:416:PRO:HD2	2.14	0.62
1:C:351:ARG:NE	1:C:351:ARG:HA	2.13	0.62
1:A:180:THR:HB	1:A:201:LEU:CD2	2.29	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:MET:CE	1:B:16:LEU:HD21	2.31	0.61
1:A:317:PHE:CE2	1:A:319:HIS:HB3	2.37	0.60
1:A:452:VAL:CG1	1:A:452:VAL:O	2.49	0.59
1:A:366:ARG:HD3	4:A:613:HOH:O	2.02	0.58
1:B:193:THR:HG23	1:B:196:GLN:H	1.68	0.58
1:C:285:LLP:H4'1	3:C:502:DAV:HT1	1.67	0.58
1:B:193:THR:HG22	1:B:196:GLN:CG	2.32	0.58
1:A:156:VAL:HG12	1:A:160:MET:HE2	1.86	0.58
1:D:51:ASP:HA	1:D:413:ILE:HB	1.86	0.58
1:D:182:PRO:HD2	1:D:226:MET:HE1	1.85	0.57
1:A:397:LEU:HD13	1:A:452:VAL:HG13	1.86	0.57
1:B:24:SER:HA	1:B:27:GLN:HB3	1.87	0.56
1:C:366:ARG:NH1	1:C:446:ASP:OD1	2.38	0.55
1:A:83:HIS:CE1	1:A:88:ARG:HH12	2.25	0.55
1:A:7:TRP:HB3	1:A:32:VAL:HG21	1.89	0.55
1:D:362:ARG:O	1:D:365:ASP:HB2	2.07	0.55
1:C:404:ALA:HB2	1:C:416:PRO:CD	2.37	0.55
1:A:415:ARG:C	1:A:415:ARG:HD3	2.27	0.54
1:C:448:VAL:O	1:C:452:VAL:HG22	2.07	0.54
1:A:180:THR:HB	1:A:201:LEU:HD22	1.88	0.54
1:A:114:THR:HG22	1:A:321:PHE:CE2	2.43	0.54
1:D:100:LEU:O	1:D:104:SER:HB3	2.09	0.53
1:A:171:LEU:HB3	1:A:172:PRO:HA	1.90	0.53
1:C:180:THR:HB	1:C:201:LEU:HD22	1.90	0.53
1:D:393:PHE:HB2	1:D:399:VAL:HG21	1.90	0.53
1:C:51:ASP:HA	1:C:413:ILE:HB	1.90	0.53
1:B:156:VAL:HG12	1:B:160:MET:HE2	1.90	0.52
1:C:415:ARG:HH11	1:C:416:PRO:HD2	1.74	0.52
1:B:259:ILE:HG12	1:B:285:LLP:O3	2.09	0.52
1:C:366:ARG:HB2	1:C:367:PRO:HD2	1.91	0.52
1:C:258:VAL:HG13	1:C:284:SER:HB3	1.91	0.52
1:C:402:ARG:NH1	4:C:655:HOH:O	2.41	0.52
1:C:321:PHE:HB2	1:C:324:SER:HB3	1.92	0.52
1:C:292:PHE:CZ	1:D:293:PRO:HD3	2.45	0.51
1:C:400:SER:HB2	1:C:416:PRO:CB	2.37	0.51
1:A:165:TYR:O	1:A:168:VAL:HG22	2.12	0.50
1:D:264:ARG:HG2	1:D:378:MET:HG3	1.94	0.50
1:C:351:ARG:HA	1:C:351:ARG:HE	1.75	0.49
1:B:157:SER:HA	1:B:160:MET:CE	2.43	0.49
1:D:253:MET:CE	1:D:276:PHE:HE2	2.22	0.49
1:D:57:TRP:HE1	1:D:415:ARG:NH1	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:322:THR:HA	1:D:56:LEU:HD23	1.94	0.48
1:D:193:THR:HG23	1:D:196:GLN:H	1.78	0.48
1:D:393:PHE:CB	1:D:399:VAL:HG21	2.44	0.48
1:C:127:MET:HE1	1:C:299:LEU:HD11	1.95	0.48
1:A:316:GLU:O	1:A:318:PRO:HD3	2.13	0.48
1:D:243:LEU:HD11	1:D:253:MET:HG2	1.95	0.47
1:A:83:HIS:HE2	1:A:88:ARG:HH12	1.62	0.47
1:B:393:PHE:HB2	1:B:399:VAL:HG11	1.95	0.47
1:C:171:LEU:HB3	1:C:172:PRO:HA	1.96	0.47
1:A:114:THR:HG22	1:A:321:PHE:HE2	1.78	0.47
1:C:40:TYR:OH	1:C:436:GLU:OE1	2.28	0.47
1:A:75:GLN:HG2	1:A:328:VAL:HA	1.97	0.47
1:C:76:TYR:CE2	1:C:328:VAL:HG11	2.50	0.47
1:C:224:PRO:O	1:C:234:PRO:HD3	2.15	0.47
1:C:307:VAL:O	1:C:311:VAL:HG23	2.15	0.47
1:A:293:PRO:HD3	1:B:292:PHE:CZ	2.49	0.47
1:B:353:ALA:N	1:B:354:PRO:HD2	2.30	0.47
1:B:27:GLN:HG3	1:B:28:ARG:HG3	1.96	0.47
1:A:88:ARG:HG2	1:B:31:VAL:HB	1.97	0.47
1:B:387:LYS:HB3	1:B:388:PRO:HD3	1.96	0.47
1:C:81:GLY:HA2	1:C:327:PRO:HG2	1.96	0.47
1:C:156:VAL:HG12	1:C:160:MET:HE2	1.97	0.46
1:B:397:LEU:HD22	1:B:452:VAL:HG22	1.96	0.46
1:D:253:MET:CE	1:D:276:PHE:CE2	2.96	0.46
1:D:131:LEU:HD11	1:D:306:ARG:HB3	1.96	0.46
1:D:58:ASN:HB3	1:D:285:LLP:HG3	1.99	0.45
1:D:147:TRP:O	1:D:148:ASN:HB2	2.16	0.45
1:B:256:ASP:CG	1:B:285:LLP:H2'2	2.36	0.45
1:B:11:ALA:O	1:B:15:SER:HB2	2.17	0.45
1:A:314:ILE:O	1:A:315:GLU:HB2	2.16	0.45
1:D:189:GLU:O	1:D:192:GLU:HB3	2.17	0.45
1:D:387:LYS:HB3	1:D:388:PRO:HD3	1.97	0.45
1:D:57:TRP:CD2	1:D:259:ILE:HD12	2.52	0.45
1:A:83:HIS:CE1	1:A:88:ARG:NH1	2.86	0.44
1:A:106:PHE:HB3	1:A:301:PRO:HD3	1.98	0.44
1:B:340:VAL:HA	1:B:345:LEU:HB2	1.99	0.44
1:A:179:LEU:HB3	1:A:204:GLU:OE1	2.18	0.44
1:B:258:VAL:HG12	1:B:285:LLP:HD3	1.99	0.44
1:C:16:LEU:HD11	1:D:307:VAL:HG11	2.00	0.43
1:C:56:LEU:O	1:C:57:TRP:HB2	2.17	0.43
1:D:24:SER:O	1:D:28:ARG:HB3	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:434:MET:O	1:B:437:MET:HB3	2.18	0.43
1:C:183:HIS:HB2	1:C:232:ILE:HG21	2.00	0.43
1:D:6:SER:O	1:D:10:ARG:HG3	2.19	0.43
1:B:156:VAL:HG12	1:B:160:MET:CE	2.49	0.43
1:A:294:MET:HE1	1:A:330:CYS:HA	2.00	0.43
1:A:366:ARG:HB2	1:A:367:PRO:HD2	2.00	0.42
1:C:323:ALA:O	1:C:326:HIS:HB2	2.20	0.42
1:D:33:VAL:HA	1:D:43:ASP:HA	2.01	0.42
1:C:415:ARG:HA	1:C:416:PRO:HD3	1.81	0.42
1:A:415:ARG:HD3	1:A:416:PRO:N	2.34	0.42
1:C:394:ASP:HB3	1:C:396:ASN:OD1	2.19	0.42
1:C:140:LYS:HA	1:C:216:THR:HA	2.02	0.42
1:C:226:MET:O	1:C:231:VAL:HA	2.19	0.42
1:B:150:TYR:HA	1:B:161:THR:HG23	2.00	0.42
1:D:182:PRO:HD2	1:D:226:MET:CE	2.50	0.42
1:D:198:VAL:HG21	1:D:236:LYS:O	2.19	0.41
1:D:146:ARG:NH2	4:D:621:HOH:O	2.52	0.41
1:B:147:TRP:O	1:B:148:ASN:CB	2.55	0.41
1:D:145:THR:HG21	1:D:160:MET:HB3	2.02	0.41
1:C:116:SER:HB3	1:D:115:ASN:ND2	2.35	0.41
1:D:193:THR:CG2	1:D:196:GLN:H	2.33	0.41
1:D:340:VAL:HA	1:D:345:LEU:HB2	2.02	0.41
1:A:389:THR:O	1:A:390:LYS:HB2	2.19	0.41
1:B:100:LEU:O	1:B:104:SER:HB3	2.20	0.41
1:C:340:VAL:HA	1:C:345:LEU:HB2	2.03	0.41
1:A:31:VAL:HB	1:B:88:ARG:HG2	2.03	0.41
1:C:380:ALA:HA	1:C:421:ILE:O	2.19	0.41
1:A:360:LEU:HD11	1:A:379:TRP:HB3	2.03	0.41
1:C:253:MET:CE	1:C:278:PRO:HB3	2.49	0.41
1:C:414:CYS:O	1:C:416:PRO:HD3	2.21	0.41
1:B:193:THR:CG2	1:B:196:GLN:H	2.32	0.41
1:B:66:LYS:O	1:B:70:GLU:HG2	2.21	0.41
1:A:226:MET:O	1:A:231:VAL:HA	2.20	0.41
1:C:165:TYR:CD2	1:D:318:PRO:HB2	2.56	0.41
1:B:193:THR:CG2	1:B:196:GLN:HG3	2.47	0.40
1:A:226:MET:HB2	1:A:232:ILE:HB	2.02	0.40
1:A:105:PRO:HD3	1:A:269:TRP:CD1	2.56	0.40
1:A:14:TYR:CE1	1:B:98:GLU:HG3	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	446/465 (96%)	425 (95%)	19 (4%)	2 (0%)	39	65
1	B	446/465 (96%)	417 (94%)	26 (6%)	3 (1%)	26	51
1	C	446/465 (96%)	424 (95%)	21 (5%)	1 (0%)	52	77
1	D	446/465 (96%)	418 (94%)	23 (5%)	5 (1%)	17	36
All	All	1784/1860 (96%)	1684 (94%)	89 (5%)	11 (1%)	30	56

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	284	SER
1	B	371	GLU
1	D	231	VAL
1	D	55	GLY
1	D	262	PHE
1	B	231	VAL
1	B	375	ILE
1	A	55	GLY
1	C	231	VAL
1	A	231	VAL
1	D	416	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	360/373 (96%)	353 (98%)	7 (2%)	65	86
1	B	360/373 (96%)	354 (98%)	6 (2%)	68	88
1	C	360/373 (96%)	350 (97%)	10 (3%)	51	78
1	D	360/373 (96%)	352 (98%)	8 (2%)	60	83
All	All	1440/1492 (96%)	1409 (98%)	31 (2%)	60	83

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	VAL
1	A	146	ARG
1	A	314	ILE
1	A	351	ARG
1	A	356	PHE
1	A	391	THR
1	A	415	ARG
1	B	103	VAL
1	B	253	MET
1	B	351	ARG
1	B	356	PHE
1	B	365	ASP
1	B	399	VAL
1	C	25	VAL
1	C	53	ASN
1	C	107	ASP
1	C	146	ARG
1	C	236	LYS
1	C	253	MET
1	C	314	ILE
1	C	356	PHE
1	C	414	CYS
1	C	415	ARG
1	D	53	ASN
1	D	146	ARG
1	D	253	MET
1	D	286	ASN
1	D	356	PHE
1	D	368	ASN
1	D	391	THR
1	D	414	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such

sidechains are listed below:

Mol	Chain	Res	Type
1	B	53	ASN
1	D	115	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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$
1	LLP	A	285	1	23,24,25	3.36	5 (21%)	28,32,34	1.91	9 (32%)
1	LLP	B	285	1	23,24,25	3.80	6 (26%)	28,32,34	1.91	8 (28%)
1	LLP	C	285	1	23,24,25	3.68	6 (26%)	28,32,34	1.82	11 (39%)
1	LLP	D	285	1	23,24,25	4.05	5 (21%)	28,32,34	1.57	6 (21%)

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
1	LLP	A	285	1	-	0/15/17/19	0/1/1/1
1	LLP	B	285	1	-	0/15/17/19	0/1/1/1
1	LLP	C	285	1	-	0/15/17/19	0/1/1/1
1	LLP	D	285	1	-	0/15/17/19	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	285	LLP	C6-C5	2.10	1.42	1.37
1	C	285	LLP	CB-CA	2.36	1.56	1.53
1	A	285	LLP	C4-C4'	2.84	1.51	1.46
1	C	285	LLP	C4-C4'	3.22	1.52	1.46
1	D	285	LLP	C4-C4'	4.00	1.53	1.46
1	B	285	LLP	C4-C4'	4.11	1.53	1.46
1	A	285	LLP	C4-C3	5.09	1.47	1.40
1	C	285	LLP	C4-C3	6.00	1.48	1.40
1	A	285	LLP	C4-C5	6.35	1.50	1.42
1	B	285	LLP	C4-C3	6.50	1.48	1.40
1	A	285	LLP	C4'-NZ	6.52	1.47	1.27
1	C	285	LLP	C4'-NZ	6.61	1.47	1.27
1	C	285	LLP	C4-C5	6.62	1.50	1.42
1	B	285	LLP	C4'-NZ	6.77	1.47	1.27
1	D	285	LLP	C4'-NZ	6.85	1.47	1.27
1	B	285	LLP	C4-C5	6.99	1.51	1.42
1	D	285	LLP	C4-C3	7.16	1.49	1.40
1	D	285	LLP	C4-C5	7.57	1.52	1.42
1	A	285	LLP	C3-C2	11.50	1.48	1.40
1	C	285	LLP	C3-C2	12.65	1.49	1.40
1	B	285	LLP	C3-C2	12.87	1.49	1.40
1	D	285	LLP	C3-C2	13.92	1.50	1.40

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	285	LLP	C3-C4-C5	-5.56	113.94	118.11
1	C	285	LLP	C4-C4'-NZ	-3.75	104.16	125.06
1	A	285	LLP	C4-C4'-NZ	-3.71	104.39	125.06
1	D	285	LLP	C3-C4-C5	-3.42	115.54	118.11
1	B	285	LLP	C2'-C2-C3	-3.41	116.92	121.04
1	B	285	LLP	C4-C4'-NZ	-3.08	107.90	125.06
1	A	285	LLP	C3-C4-C4'	-2.90	116.40	120.16
1	C	285	LLP	C2'-C2-C3	-2.82	117.64	121.04
1	D	285	LLP	C4-C4'-NZ	-2.75	109.77	125.06
1	C	285	LLP	C3-C4-C5	-2.60	116.16	118.11
1	A	285	LLP	C3-C4-C5	-2.40	116.31	118.11
1	C	285	LLP	O-C-CA	-2.36	119.34	125.49
1	C	285	LLP	OP3-P-OP4	-2.32	99.89	106.56
1	B	285	LLP	OP2-P-OP4	-2.30	99.95	106.56
1	B	285	LLP	O-C-CA	-2.30	119.51	125.49
1	A	285	LLP	OP3-P-OP4	-2.13	100.42	106.56
1	C	285	LLP	O3-C3-C2	2.05	121.22	117.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	285	LLP	O3-C3-C2	2.06	121.24	117.66
1	C	285	LLP	OP3-P-OP2	2.07	115.26	107.38
1	B	285	LLP	CD-CE-NZ	2.10	114.41	110.98
1	C	285	LLP	OP3-P-OP1	2.12	117.39	110.58
1	A	285	LLP	OP3-P-OP2	2.18	115.70	107.38
1	D	285	LLP	CD-CE-NZ	2.25	114.66	110.98
1	B	285	LLP	CE-NZ-C4'	2.51	126.22	118.97
1	A	285	LLP	O3-C3-C2	2.56	122.11	117.66
1	D	285	LLP	OP3-P-OP2	2.58	117.22	107.38
1	A	285	LLP	CE-NZ-C4'	2.61	126.51	118.97
1	C	285	LLP	OP4-C5'-C5	2.90	113.79	108.99
1	B	285	LLP	OP3-P-OP2	2.91	118.47	107.38
1	C	285	LLP	C5-C4-C4'	3.06	125.91	121.52
1	D	285	LLP	C5-C4-C4'	3.17	126.07	121.52
1	C	285	LLP	CE-NZ-C4'	3.42	128.86	118.97
1	A	285	LLP	OP4-C5'-C5	3.69	115.10	108.99
1	A	285	LLP	C5-C4-C4'	3.99	127.25	121.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	285	LLP	5	0
1	C	285	LLP	2	0
1	D	285	LLP	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	DAV	A	502	-	4,7,7	0.37	0	4,7,7	0.88	0
3	DAV	C	502	-	4,7,7	0.28	0	4,7,7	0.94	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
3	DAV	A	502	-	-	0/3/5/5	0/0/0/0
3	DAV	C	502	-	-	0/3/5/5	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	502	DAV	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	448/465 (96%)	-0.55	2 (0%) 93 91	16, 32, 56, 82	2 (0%)
1	B	448/465 (96%)	-0.45	11 (2%) 61 54	16, 33, 67, 85	3 (0%)
1	C	448/465 (96%)	-0.56	2 (0%) 93 91	21, 34, 55, 75	4 (0%)
1	D	448/465 (96%)	-0.37	10 (2%) 65 59	22, 40, 71, 88	4 (0%)
All	All	1792/1860 (96%)	-0.48	25 (1%) 78 74	16, 34, 67, 88	13 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	23	PRO	4.9
1	D	27	GLN	4.5
1	B	27	GLN	3.5
1	D	23	PRO	3.4
1	B	26	HIS	3.3
1	B	388	PRO	3.2
1	B	5	GLN	2.8
1	D	453	ALA	2.8
1	D	190	GLU	2.7
1	D	26	HIS	2.5
1	B	191	GLY	2.5
1	C	247	ARG	2.5
1	A	388	PRO	2.5
1	B	24	SER	2.5
1	B	190	GLU	2.3
1	B	25	VAL	2.3
1	D	29	GLY	2.2
1	A	453	ALA	2.2
1	B	395	ALA	2.1
1	D	396	ASN	2.1
1	D	275	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	389	THR	2.0
1	D	452	VAL	2.0
1	D	395	ALA	2.0
1	C	396	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	LLP	B	285	24/25	0.92	0.17	-	34,48,52,56	0
1	LLP	C	285	24/25	0.96	0.12	-	33,38,41,42	0
1	LLP	A	285	24/25	0.97	0.11	-	31,32,33,34	0
1	LLP	D	285	24/25	0.92	0.18	-	39,50,54,56	0

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	DAV	A	502	8/8	0.78	0.25	6.61	34,45,60,63	0
3	DAV	C	502	8/8	0.87	0.20	4.91	54,57,63,66	0
2	NA	C	501	1/1	0.53	0.14	-0.30	48,48,48,48	0
2	NA	D	501	1/1	0.93	0.09	-0.87	26,26,26,26	0
2	NA	B	501	1/1	0.93	0.08	-1.27	29,29,29,29	0
2	NA	A	501	1/1	0.96	0.08	-1.28	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.