Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:24 PM GMT

PDB ID	:	4EQ4
Title	:	Crystal structure of seleno-methionine derivatized GH3.12
Authors	:	Zubieta, C.; Nanao, M.; Jez, J.; Westfall, C.; Kapp, U.
Deposited on	:	2012-04-18
Resolution	:	2.07 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:

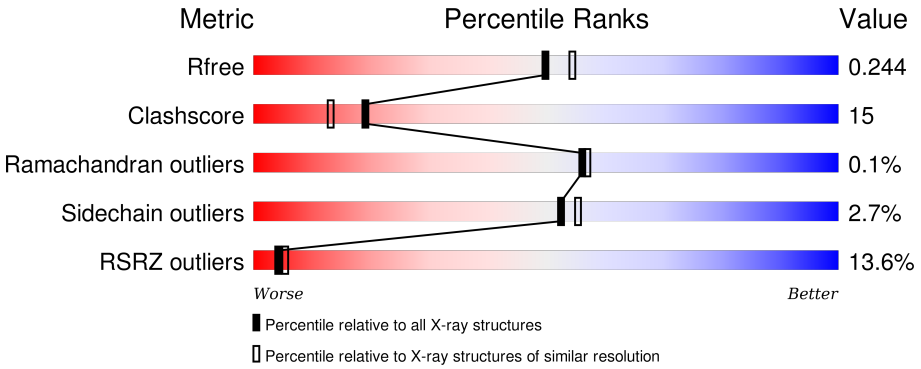
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.07 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	4546 (2.10-2.06)
Clashscore	102246	5101 (2.10-2.06)
Ramachandran outliers	100387	5048 (2.10-2.06)
Sidechain outliers	100360	5049 (2.10-2.06)
RSRZ outliers	91569	4556 (2.10-2.06)

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	581	13% 72% 20% • 6%
1	B	581	12% 73% 18% • 9%

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
2	SAL	B	601	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9183 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.

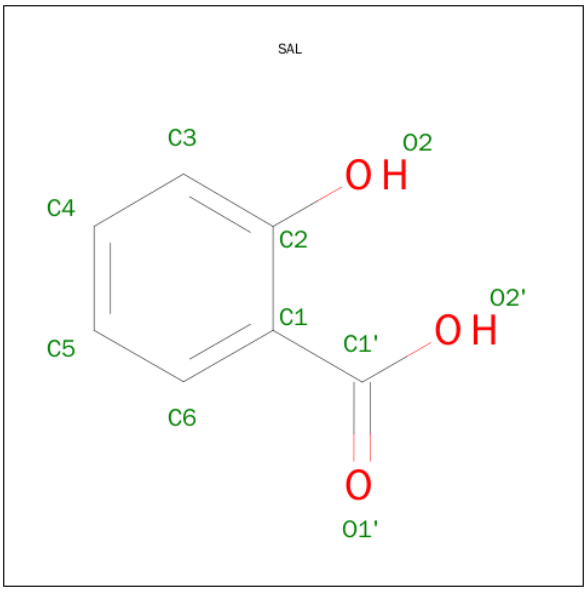
- Molecule 1 is a protein called 4-substituted benzoates-glutamate ligase GH3.12.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	545	Total	C	N	O	S	Se	0	6	0
			4277	2717	701	831	13	15			
1	B	531	Total	C	N	O	S	Se	0	6	0
			4177	2656	683	810	14	14			

There are 12 discrepancies between the modelled and reference sequences:

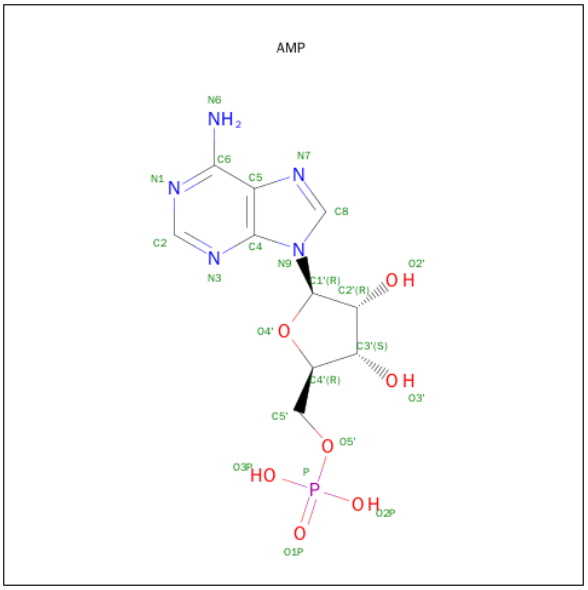
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	EXPRESSION TAG	UNP Q9LYU4
A	-4	SER	-	EXPRESSION TAG	UNP Q9LYU4
A	-3	HIS	-	EXPRESSION TAG	UNP Q9LYU4
A	-2	MSE	-	EXPRESSION TAG	UNP Q9LYU4
A	-1	ALA	-	EXPRESSION TAG	UNP Q9LYU4
A	0	SER	-	EXPRESSION TAG	UNP Q9LYU4
B	-5	GLY	-	EXPRESSION TAG	UNP Q9LYU4
B	-4	SER	-	EXPRESSION TAG	UNP Q9LYU4
B	-3	HIS	-	EXPRESSION TAG	UNP Q9LYU4
B	-2	MSE	-	EXPRESSION TAG	UNP Q9LYU4
B	-1	ALA	-	EXPRESSION TAG	UNP Q9LYU4
B	0	SER	-	EXPRESSION TAG	UNP Q9LYU4

- Molecule 2 is 2-HYDROXYBENZOIC ACID (three-letter code: SAL) (formula: $C_7H_6O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 10 7 3	0	0
2	B	1	Total C O 10 7 3	0	0

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 23 10 5 7 1	0	0
3	B	1	Total C N O P 23 10 5 7 1	0	0

- Molecule 4 is water.

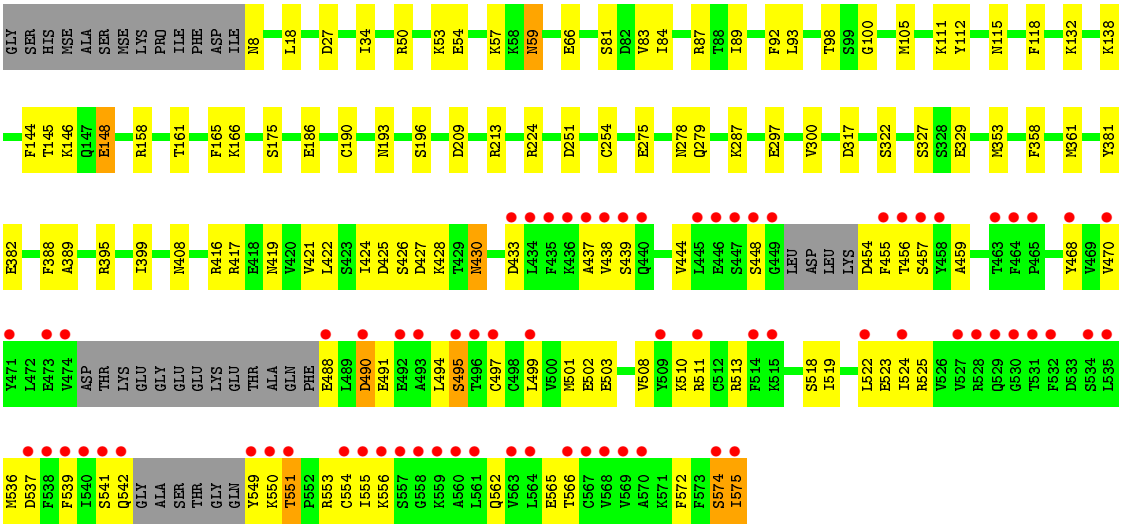
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	351	Total O 351 351	0	0
4	B	312	Total O 312 312	0	0

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.

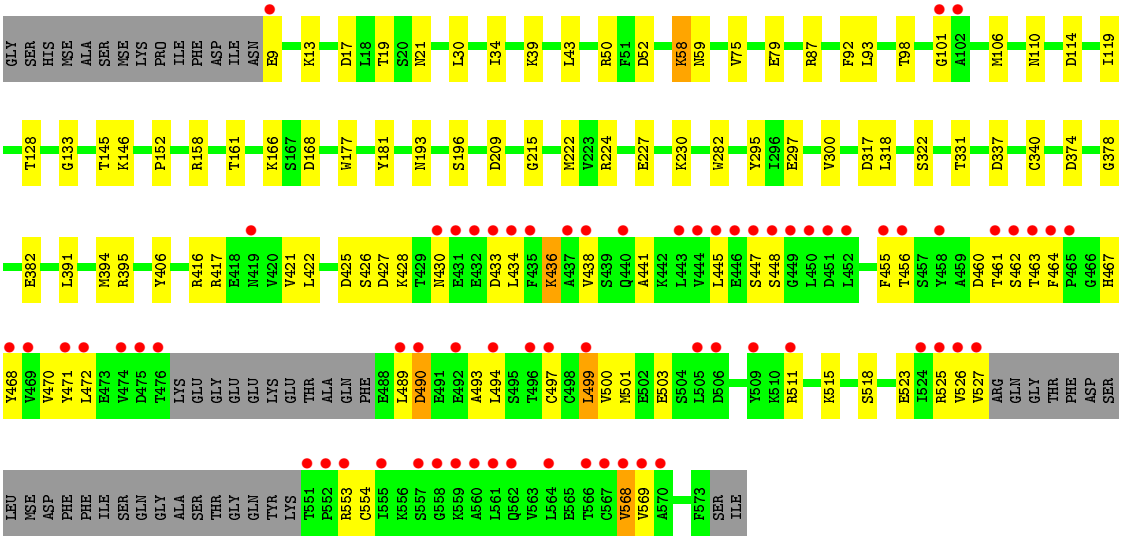
- Molecule 1: 4-substituted benzoates-glutamate ligase GH3.12

Chain A:



- Molecule 1: 4-substituted benzoates-glutamate ligase GH3.12

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	90.86Å 66.30Å 100.45Å 90.00° 106.63° 90.00°	Depositor
Resolution (Å)	56.97 – 2.07 56.96 – 2.08	Depositor EDS
% Data completeness (in resolution range)	99.1 (56.97-2.07) 99.1 (56.96-2.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.25	Depositor
$< I/\sigma(I) >$ [1]	1.46 (at 2.08Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.214 , 0.252 0.208 , 0.244	Depositor DCC
R_{free} test set	3501 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	20.7	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 48.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 68898 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9183	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% 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: AMP, SAL

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	0.66	1/4366 (0.0%)	0.69	0/5896
1	B	0.66	0/4266	0.69	1/5767 (0.0%)
All	All	0.66	1/8632 (0.0%)	0.69	1/11663 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	81	SER	CB-OG	-5.37	1.35	1.42

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	110	ASN	CB-CA-C	-5.65	99.09	110.40

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	4277	0	4119	159	1
1	B	4177	0	4062	113	1
2	A	10	0	5	0	0
2	B	10	0	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	23	0	12	0	0
3	B	23	0	12	0	0
4	A	351	0	0	34	0
4	B	312	0	0	27	0
All	All	9183	0	8215	255	1

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 15.

All (255) 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:438:VAL:CG2	1:A:501:MSE:HE1	1.27	1.56
1:B:455:PHE:CB	1:B:553:ARG:HH12	1.23	1.46
1:A:438:VAL:CG2	1:A:501:MSE:CE	1.97	1.41
1:A:438:VAL:HG22	1:A:501:MSE:CE	1.64	1.23
1:A:438:VAL:HG23	1:A:501:MSE:CE	1.61	1.22
1:A:146:LYS:HE2	1:A:511:ARG:NH2	1.52	1.22
1:B:455:PHE:CB	1:B:553:ARG:NH1	2.06	1.17
1:A:502:GLU:HG3	1:A:522:LEU:HD12	1.22	1.14
1:A:510:LYS:HZ1	1:B:499:LEU:HD13	1.02	1.11
1:A:502:GLU:CG	1:A:522:LEU:HD12	1.82	1.09
1:A:510:LYS:NZ	1:B:499:LEU:HD13	1.69	1.08
1:B:438:VAL:HG21	1:B:553:ARG:HH22	1.19	1.07
1:A:438:VAL:HG23	1:A:501:MSE:HE1	1.07	1.06
1:A:499:LEU:HD21	1:A:575:ILE:H	1.19	1.06
1:B:317:ASP:C	4:B:952:HOH:O	1.95	1.05
1:B:438:VAL:HG21	1:B:553:ARG:NH2	1.70	1.05
1:A:468:TYR:HB2	1:A:522:LEU:HD23	1.34	1.04
1:A:416:ARG:CZ	4:A:1018:HOH:O	2.04	1.04
1:B:87:ARG:NH2	4:B:773:HOH:O	1.92	1.02
1:A:575:ILE:HD12	1:B:515:LYS:HD2	1.38	1.02
1:A:438:VAL:HG22	1:A:501:MSE:HE1	1.15	1.01
1:B:9:GLU:N	4:B:822:HOH:O	1.92	1.01
1:A:499:LEU:HD21	1:A:575:ILE:N	1.74	1.01
1:A:98:THR:O	4:A:1035:HOH:O	1.81	0.98
1:A:416:ARG:NE	4:A:1018:HOH:O	1.93	0.97
1:A:536:MSE:HG3	1:A:549:TYR:CD2	1.99	0.96
1:A:468:TYR:HB2	1:A:522:LEU:CD2	1.97	0.95
1:A:146:LYS:HE2	1:A:511:ARG:HH22	1.29	0.91
1:B:317:ASP:O	4:B:952:HOH:O	1.83	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:ASP:OD2	4:B:992:HOH:O	1.88	0.91
1:B:318:LEU:N	4:B:952:HOH:O	2.00	0.91
1:A:146:LYS:HE2	1:A:511:ARG:HH21	1.37	0.90
1:A:408:ASN:OD1	4:A:794:HOH:O	1.90	0.90
1:B:79:GLU:OE1	4:B:993:HOH:O	1.91	0.89
1:A:438:VAL:CG2	1:A:501:MSE:HE3	1.99	0.89
1:B:58:LYS:HG2	1:B:59:ASN:OD1	1.72	0.88
1:A:499:LEU:CD2	1:A:575:ILE:H	1.85	0.88
1:A:468:TYR:CB	1:A:522:LEU:HD23	2.05	0.87
1:A:317:ASP:O	4:A:1019:HOH:O	1.92	0.86
1:B:318:LEU:CA	4:B:952:HOH:O	2.24	0.86
1:A:575:ILE:HD12	1:B:515:LYS:CD	2.05	0.85
1:B:455:PHE:C	1:B:553:ARG:NH1	2.30	0.85
1:A:287:LYS:HE2	4:A:1037:HOH:O	1.77	0.84
1:B:318:LEU:HA	4:B:952:HOH:O	1.77	0.83
1:B:455:PHE:CA	1:B:553:ARG:NH1	2.40	0.83
1:A:510:LYS:NZ	1:B:499:LEU:HD22	1.92	0.83
1:A:146:LYS:NZ	4:A:947:HOH:O	2.13	0.82
1:B:374:ASP:OD2	4:B:983:HOH:O	1.97	0.82
1:A:499:LEU:HD23	1:A:574:SER:OG	1.80	0.81
1:B:455:PHE:CA	1:B:553:ARG:HH12	1.92	0.81
1:A:27:ASP:OD1	1:A:53:LYS:NZ	2.12	0.81
1:A:100:GLY:O	4:A:993:HOH:O	1.98	0.81
1:B:489:LEU:O	1:B:490:ASP:CB	2.30	0.80
1:B:114:ASP:HB2	4:B:986:HOH:O	1.83	0.79
1:A:455:PHE:HE1	1:A:553:ARG:HD2	1.48	0.79
1:A:209:ASP:OD1	4:A:987:HOH:O	2.00	0.78
1:A:438:VAL:CA	1:A:501:MSE:HE3	2.13	0.78
1:A:327:SER:O	4:A:1027:HOH:O	2.00	0.78
1:A:66[B]:GLU:OE2	4:A:976:HOH:O	1.98	0.77
1:A:287:LYS:NZ	4:A:922:HOH:O	2.18	0.76
1:A:510:LYS:NZ	1:B:499:LEU:CD1	2.48	0.75
1:A:499:LEU:HD21	1:A:575:ILE:CA	2.16	0.75
1:A:510:LYS:HZ3	1:B:499:LEU:HD22	1.50	0.74
1:A:287:LYS:CE	4:A:1037:HOH:O	2.34	0.74
1:A:499:LEU:HD11	1:A:575:ILE:O	1.87	0.74
1:A:275:GLU:OE2	1:A:279:GLN:NE2	2.21	0.74
1:A:213:ARG:NH1	1:A:297:GLU:OE1	2.21	0.73
1:B:224[B]:ARG:NH1	4:B:929:HOH:O	2.22	0.73
1:B:470:VAL:HG12	1:B:472:LEU:HD13	1.72	0.72
1:A:419:ASN:OD1	4:A:815:HOH:O	2.07	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:VAL:HG23	1:B:422:LEU:HG	1.71	0.71
1:A:565:GLU:HA	4:A:1028:HOH:O	1.89	0.71
1:A:455:PHE:CE1	1:A:553:ARG:HD2	2.25	0.71
1:A:536:MSE:HG3	1:A:549:TYR:CE2	2.26	0.71
1:B:455:PHE:C	1:B:553:ARG:HH11	1.93	0.71
1:A:499:LEU:HD11	1:A:575:ILE:C	2.11	0.70
1:A:424:ILE:HD11	1:A:459:ALA:HB1	1.73	0.70
1:A:317:ASP:C	4:A:1019:HOH:O	2.28	0.70
1:A:468:TYR:CB	1:A:522:LEU:CD2	2.66	0.70
1:A:457:SER:OG	1:A:553:ARG:O	2.10	0.70
1:A:502:GLU:HG3	1:A:522:LEU:CD1	2.12	0.69
1:A:416:ARG:NH2	4:A:1018:HOH:O	2.20	0.69
1:A:382:GLU:OE1	1:A:395:ARG:NH2	2.26	0.68
1:A:438:VAL:HA	1:A:501:MSE:HE3	1.74	0.67
1:A:287:LYS:NZ	4:A:1037:HOH:O	2.26	0.67
1:B:300:VAL:HG22	1:B:322:SER:HB2	1.77	0.67
1:B:19:THR:OG1	4:B:897:HOH:O	1.85	0.66
1:B:427:ASP:OD2	1:B:468:TYR:OH	2.09	0.66
1:A:497:CYS:O	1:A:501:MSE:HG3	1.94	0.66
1:A:551:THR:HG22	1:A:553:ARG:NH1	2.11	0.65
1:B:526:VAL:O	1:B:568:VAL:HA	1.96	0.65
1:B:50:ARG:NE	4:B:873:HOH:O	2.24	0.65
1:B:422:LEU:HD13	1:B:468:TYR:CD2	2.32	0.64
1:A:427:ASP:OD1	1:A:519:ILE:HD11	1.97	0.64
1:B:455:PHE:O	1:B:553:ARG:NH1	2.29	0.63
1:A:438:VAL:N	1:A:501:MSE:HE3	2.14	0.63
1:B:421:VAL:HB	1:B:554:CYS:HB2	1.80	0.63
1:A:437:ALA:HB1	1:A:501:MSE:HA	1.80	0.63
1:A:510:LYS:HZ1	1:B:499:LEU:CD1	1.94	0.62
1:B:434:LEU:O	1:B:434:LEU:HD12	1.99	0.62
1:A:470:VAL:CG1	1:A:524:ILE:HG12	2.28	0.62
1:B:224[B]:ARG:HG3	1:B:464:PHE:HZ	1.63	0.62
1:A:551:THR:HG22	1:A:553:ARG:HH11	1.64	0.62
1:A:148:GLU:OE1	1:A:158:ARG:NH2	2.31	0.62
1:A:87:ARG:NH2	4:A:819:HOH:O	2.31	0.60
1:B:489:LEU:CB	1:B:494:LEU:HD11	2.31	0.60
1:B:119:ILE:HG13	1:B:331:THR:HG21	1.83	0.60
1:A:424:ILE:O	1:A:427:ASP:OD1	2.18	0.60
1:A:161[B]:THR:HB	4:A:924:HOH:O	2.02	0.59
1:A:422:LEU:HD21	1:A:457:SER:HB2	1.85	0.59
1:B:568:VAL:O	1:B:568:VAL:HG22	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:ASP:N	1:A:490:ASP:OD2	2.28	0.59
1:A:502:GLU:HG2	1:A:522:LEU:HD12	1.80	0.58
1:A:146:LYS:CE	1:A:511:ARG:HH21	2.13	0.58
1:A:456:THR:OG1	1:A:457:SER:N	2.37	0.58
1:A:224[A]:ARG:HD2	4:A:986:HOH:O	2.03	0.58
1:A:510:LYS:NZ	1:B:499:LEU:CD2	2.64	0.57
1:B:168:ASP:OD1	4:B:996:HOH:O	2.17	0.57
1:A:83:VAL:HG12	1:A:84:ILE:HG23	1.86	0.57
1:A:224[B]:ARG:HD2	4:A:986:HOH:O	2.04	0.57
1:B:470:VAL:HG12	1:B:472:LEU:CD1	2.34	0.57
1:B:161[B]:THR:HG23	4:B:714:HOH:O	2.03	0.57
1:A:494:LEU:HD22	1:A:572:PHE:CE2	2.40	0.57
1:A:562:GLN:O	1:A:566:THR:HG23	2.05	0.57
1:A:161[B]:THR:HG22	4:A:720:HOH:O	2.02	0.57
1:A:224[B]:ARG:NH1	4:A:995:HOH:O	2.37	0.57
1:A:190:CYS:HB3	1:A:196:SER:HB3	1.86	0.57
1:A:224[A]:ARG:NH1	4:A:995:HOH:O	2.38	0.56
1:B:499:LEU:CD1	1:B:503:GLU:OE2	2.53	0.56
1:A:111:LYS:HG2	1:A:388:PHE:CG	2.40	0.56
1:A:510:LYS:HZ2	1:B:499:LEU:HD22	1.69	0.56
1:A:144:PHE:HB3	1:A:193:ASN:ND2	2.21	0.56
1:B:445:LEU:O	1:B:448:SER:N	2.39	0.56
1:A:112:TYR:OH	4:A:1027:HOH:O	2.17	0.55
1:A:425:ASP:CG	1:A:426:SER:H	2.10	0.55
1:B:30:LEU:O	1:B:34:ILE:HG12	2.06	0.55
1:A:209:ASP:OD2	4:A:981:HOH:O	2.18	0.55
1:B:499:LEU:CD1	1:B:503:GLU:CD	2.75	0.55
1:A:213:ARG:NE	4:A:921:HOH:O	2.31	0.55
1:B:417:ARG:HD3	1:B:428:LYS:HD3	1.88	0.55
1:B:499:LEU:C	1:B:499:LEU:HD12	2.28	0.54
1:A:146:LYS:CE	1:A:511:ARG:NH2	2.47	0.54
1:A:18:LEU:HD11	1:A:118:PHE:HZ	1.72	0.54
1:A:575:ILE:CD1	1:B:515:LYS:CD	2.82	0.53
1:B:430:ASN:OD1	1:B:433:ASP:N	2.42	0.53
1:B:499:LEU:HG	1:B:500:VAL:N	2.24	0.53
1:B:406:TYR:HE2	4:B:897:HOH:O	1.91	0.53
1:B:224[B]:ARG:HH11	1:B:518:SER:HB3	1.73	0.53
1:A:455:PHE:CE1	1:A:553:ARG:CD	2.92	0.52
1:A:424:ILE:CD1	1:A:459:ALA:HB1	2.39	0.52
1:A:275:GLU:O	1:A:275:GLU:OE2	2.27	0.52
1:A:499:LEU:HD21	1:A:575:ILE:C	2.31	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:ILE:HD11	1:B:511:ARG:HA	1.92	0.52
1:A:502:GLU:CG	1:A:522:LEU:CD1	2.73	0.51
1:B:499:LEU:HD13	1:B:503:GLU:OE2	2.11	0.51
1:A:361:MSE:HG3	1:A:399:ILE:HD12	1.93	0.51
1:A:575:ILE:HD13	1:B:511:ARG:NE	2.25	0.51
1:B:224[B]:ARG:CZ	4:B:929:HOH:O	2.58	0.50
1:A:327:SER:OG	1:A:329:GLU:OE1	2.21	0.50
1:A:438:VAL:HG22	1:A:501:MSE:HE3	1.73	0.50
1:B:230:LYS:HE3	1:B:282:TRP:CD1	2.47	0.50
1:A:421:VAL:HB	1:A:554:CYS:HB3	1.93	0.50
1:B:227:GLU:HG3	1:B:464:PHE:CD1	2.46	0.49
1:A:554:CYS:O	1:A:555:ILE:HD13	2.13	0.49
1:B:378:GLY:HA2	4:B:798:HOH:O	2.13	0.49
1:B:224[B]:ARG:HG3	1:B:464:PHE:CZ	2.44	0.49
1:B:470:VAL:HG11	1:B:501:MSE:HE1	1.93	0.49
1:B:525:ARG:NH2	4:B:959:HOH:O	2.46	0.48
1:A:89:ILE:HD11	1:A:389:ALA:O	2.13	0.48
1:B:133:GLY:HA2	4:B:990:HOH:O	2.12	0.48
1:A:145:THR:HG21	1:A:166:LYS:HD3	1.95	0.48
1:B:441:ALA:O	1:B:445:LEU:HB2	2.13	0.48
1:A:502:GLU:OE2	1:A:513:ARG:NE	2.28	0.48
1:A:438:VAL:HG22	1:A:501:MSE:SE	2.61	0.48
1:B:295:TYR:CE1	1:B:297:GLU:HB2	2.48	0.48
1:A:536:MSE:HA	1:A:549:TYR:CZ	2.49	0.47
1:A:382:GLU:OE2	1:A:395:ARG:HB3	2.13	0.47
1:B:391:LEU:HD13	1:B:394:MSE:HE2	1.96	0.47
1:B:467:HIS:HE1	1:B:523:GLU:OE1	1.97	0.47
1:B:58:LYS:CG	1:B:59:ASN:OD1	2.54	0.47
1:A:132:LYS:HB3	4:A:975:HOH:O	2.13	0.47
1:B:21:ASN:ND2	4:B:808:HOH:O	2.39	0.47
1:A:146:LYS:HE3	1:A:193:ASN:ND2	2.30	0.47
1:A:503:GLU:HB3	1:B:503:GLU:CD	2.35	0.47
1:B:145:THR:HG21	1:B:166:LYS:HD3	1.96	0.47
1:B:445:LEU:HD13	1:B:497:CYS:SG	2.54	0.47
1:A:510:LYS:NZ	1:B:499:LEU:CG	2.78	0.47
1:A:430:ASN:ND2	1:A:433:ASP:OD2	2.48	0.47
1:A:358:PHE:HB3	1:A:381:TYR:HB3	1.98	0.46
1:B:215:GLY:HA2	1:B:222:MSE:SE	2.65	0.46
1:B:497:CYS:O	1:B:501:MSE:HG3	2.15	0.46
1:B:106:MSE:SE	1:B:394:MSE:HE1	2.64	0.46
1:A:508:VAL:O	1:A:511:ARG:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:TYR:CB	1:A:522:LEU:HD21	2.45	0.45
1:A:537:ASP:O	1:A:541:SER:N	2.32	0.45
1:A:575:ILE:HG23	1:B:511:ARG:HH21	1.81	0.45
1:B:75:VAL:HG12	1:B:92:PHE:HZ	1.81	0.45
1:B:471:TYR:HA	1:B:525:ARG:O	2.17	0.45
1:A:300:VAL:HG22	1:A:322:SER:HB2	1.99	0.45
1:A:132:LYS:HA	1:A:132:LYS:HD3	1.81	0.45
1:B:526:VAL:O	1:B:568:VAL:CA	2.64	0.44
1:B:436:LYS:HD3	1:B:436:LYS:HA	1.72	0.44
1:A:523:GLU:CD	1:A:525:ARG:HE	2.19	0.44
1:A:34:ILE:HA	1:A:34:ILE:HD13	1.82	0.44
1:A:490:ASP:HB3	1:B:152:PRO:HD3	1.99	0.44
1:A:417:ARG:HD3	1:A:428:LYS:HD3	1.99	0.44
1:B:13:LYS:HD3	1:B:17:ASP:OD1	2.17	0.44
1:B:490:ASP:O	1:B:494:LEU:HD12	2.18	0.44
1:B:499:LEU:HD12	1:B:503:GLU:CD	2.38	0.43
1:A:575:ILE:HD13	1:B:511:ARG:HE	1.83	0.43
1:A:470:VAL:HG13	1:A:524:ILE:HG12	1.98	0.43
1:A:93:LEU:HA	1:A:158:ARG:O	2.18	0.43
1:A:161[B]:THR:HG23	1:A:165:PHE:CE2	2.52	0.43
1:B:128[B]:THR:HG23	1:B:177:TRP:CZ2	2.54	0.43
1:B:374:ASP:OD2	4:B:797:HOH:O	2.21	0.43
1:B:417:ARG:NH2	4:B:735:HOH:O	2.50	0.43
1:A:138:LYS:HE2	4:A:916:HOH:O	2.19	0.43
1:B:527:VAL:HA	1:B:568:VAL:HA	1.99	0.43
1:A:186:GLU:N	1:A:186:GLU:OE1	2.45	0.43
1:A:454:ASP:OD1	1:A:455:PHE:N	2.49	0.43
1:A:536:MSE:HA	1:A:549:TYR:CE2	2.53	0.43
1:A:53:LYS:HE3	1:A:57:LYS:HE2	2.00	0.43
1:A:539:PHE:HA	1:A:542:GLN:HB2	2.01	0.43
1:A:92:PHE:HB3	1:A:105:MSE:HG2	2.01	0.43
1:A:502:GLU:HG3	1:A:522:LEU:HB2	2.00	0.43
1:B:93:LEU:HA	1:B:158:ARG:O	2.20	0.42
1:A:444:VAL:O	1:A:448:SER:HB2	2.19	0.42
1:A:132:LYS:HE3	4:A:909:HOH:O	2.20	0.42
1:A:251:ASP:OD2	1:A:254:CYS:N	2.44	0.42
1:A:499:LEU:HB3	1:A:503:GLU:OE2	2.20	0.42
1:B:460:ASP:CG	1:B:462:SER:HG	2.22	0.42
1:B:472:LEU:HA	1:B:472:LEU:HD12	1.76	0.42
1:B:181:TYR:OH	4:B:879:HOH:O	2.15	0.42
1:B:98:THR:OG1	1:B:101:GLY:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:MSE:HG3	1:A:399:ILE:CD1	2.50	0.42
1:A:575:ILE:CD1	1:B:515:LYS:HD3	2.49	0.42
1:A:115:ASN:HB3	1:A:353:MSE:SE	2.70	0.42
1:A:549:TYR:CG	1:A:550:LYS:N	2.87	0.41
1:B:382:GLU:OE2	1:B:395:ARG:HB3	2.21	0.41
1:A:491:GLU:O	1:A:495:SER:HB2	2.20	0.41
1:B:425:ASP:CG	1:B:426:SER:H	2.24	0.41
1:A:100:GLY:N	4:A:1015:HOH:O	2.52	0.41
1:B:43:LEU:HD23	1:B:43:LEU:HA	1.82	0.41
1:A:59:ASN:ND2	4:A:859:HOH:O	2.18	0.41
1:B:416:ARG:NE	4:B:909:HOH:O	2.46	0.41
1:A:224[B]:ARG:NH1	1:A:518:SER:HB3	2.36	0.41
1:B:456:THR:O	1:B:471:TYR:N	2.54	0.40
1:B:193:ASN:HA	1:B:196:SER:OG	2.21	0.40
1:B:493:ALA:HB3	1:B:494:LEU:HD12	2.02	0.40
1:A:224[B]:ARG:HD3	1:A:224[B]:ARG:HH11	1.77	0.40
1:A:491:GLU:O	1:A:491:GLU:HG2	2.22	0.40
1:A:224[A]:ARG:HH11	1:A:224[A]:ARG:HD3	1.77	0.40
1:B:337:ASP:OD2	1:B:340:CYS:HB3	2.21	0.40

All (1) 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:A:50:ARG:NH1	1:B:209:ASP:OD2[1_655]	1.78	0.42

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	543/581 (94%)	522 (96%)	21 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	531/581 (91%)	515 (97%)	15 (3%)	1 (0%)	52 52
All	All	1074/1162 (92%)	1037 (97%)	36 (3%)	1 (0%)	56 57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	490	ASP

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	472/510 (92%)	457 (97%)	15 (3%)	46 48
1	B	469/510 (92%)	459 (98%)	10 (2%)	61 65
All	All	941/1020 (92%)	916 (97%)	25 (3%)	52 55

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	54	GLU
1	A	59	ASN
1	A	148	GLU
1	A	175	SER
1	A	278	ASN
1	A	430	ASN
1	A	439	SER
1	A	488	GLU
1	A	490	ASP
1	A	495	SER
1	A	551	THR
1	A	556	LYS
1	A	574	SER
1	A	575	ILE

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Mol	Chain	Res	Type
1	B	39	LYS
1	B	58	LYS
1	B	146	LYS
1	B	436	LYS
1	B	447	SER
1	B	461	THR
1	B	463	THR
1	B	499	LEU
1	B	568	VAL
1	B	569	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	193	ASN
1	A	247	ASN
1	B	110	ASN
1	B	467	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

4 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	SAL	A	601	-	7,10,10	0.55	0	10,13,13	1.22	1 (10%)
3	AMP	A	602	-	20,25,25	0.85	1 (5%)	22,38,38	1.90	5 (22%)
2	SAL	B	601	-	7,10,10	0.73	0	10,13,13	0.79	0
3	AMP	B	602	-	20,25,25	0.85	1 (5%)	22,38,38	1.93	4 (18%)

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	SAL	A	601	-	-	0/0/4/4	0/1/1/1
3	AMP	A	602	-	-	0/6/26/26	0/3/3/3
2	SAL	B	601	-	-	0/0/4/4	0/1/1/1
3	AMP	B	602	-	-	0/6/26/26	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	AMP	C5-C4	2.78	1.46	1.40
3	B	602	AMP	C5-C4	2.87	1.47	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	602	AMP	N3-C2-N1	-6.88	123.63	128.89
3	A	602	AMP	N3-C2-N1	-6.70	123.76	128.89
2	A	601	SAL	C2-C1-C1'	-3.22	118.30	121.60
3	B	602	AMP	C1'-N9-C4	-3.15	122.19	126.94
3	A	602	AMP	C1'-N9-C4	-2.47	123.21	126.94
3	B	602	AMP	C2'-C1'-N9	-2.27	110.83	114.29
3	A	602	AMP	N6-C6-N1	2.17	123.86	119.20
3	A	602	AMP	C2-N1-C6	2.21	122.71	118.77
3	A	602	AMP	O2P-P-O1P	2.48	118.55	110.58
3	B	602	AMP	O2P-P-O1P	2.48	118.58	110.58

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	530/581 (91%)	0.59	73 (13%) 4 5	10, 21, 88, 114	0
1	B	517/581 (88%)	0.68	69 (13%) 4 6	14, 26, 93, 112	0
All	All	1047/1162 (90%)	0.63	142 (13%) 4 5	10, 24, 91, 114	0

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	541	SER	10.9
1	B	475	ASP	9.8
1	B	559	LYS	9.7
1	A	532	PHE	9.5
1	B	489	LEU	9.4
1	B	452	LEU	9.1
1	B	560	ALA	9.0
1	B	449	GLY	8.7
1	B	434	LEU	8.3
1	B	476	THR	8.3
1	B	555	ILE	8.1
1	A	540	ILE	8.1
1	B	450	LEU	7.8
1	A	539	PHE	7.7
1	A	558	GLY	7.5
1	A	435	PHE	7.4
1	A	549	TYR	7.0
1	B	564	LEU	6.4
1	B	451	ASP	6.3
1	A	448	SER	6.2
1	A	527	VAL	6.1
1	B	569	VAL	6.1
1	A	455	PHE	6.1
1	B	568	VAL	6.1

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Mol	Chain	Res	Type	RSRZ
1	A	564	LEU	6.0
1	A	551	THR	5.9
1	A	535	LEU	5.9
1	B	474	VAL	5.8
1	B	463	THR	5.8
1	A	456	THR	5.8
1	B	438	VAL	5.7
1	B	445	LEU	5.7
1	B	494	LEU	5.6
1	A	474	VAL	5.6
1	A	575	ILE	5.5
1	A	568	VAL	5.4
1	A	566	THR	5.3
1	A	463	THR	5.2
1	B	437	ALA	5.1
1	A	560	ALA	5.0
1	B	558	GLY	5.0
1	B	499	LEU	5.0
1	A	538	PHE	4.9
1	B	471	TYR	4.9
1	A	557	SER	4.9
1	B	566	THR	4.8
1	B	455	PHE	4.8
1	A	449	GLY	4.7
1	B	443	LEU	4.6
1	B	567	CYS	4.6
1	A	550	LYS	4.5
1	B	557	SER	4.5
1	A	446	GLU	4.5
1	A	497	CYS	4.4
1	B	526	VAL	4.4
1	A	567	CYS	4.4
1	B	561	LEU	4.3
1	B	465	PRO	4.3
1	B	458	TYR	4.2
1	A	438	VAL	4.2
1	A	522	LEU	4.2
1	A	530	GLY	4.2
1	B	444	VAL	4.2
1	B	435	PHE	4.1
1	A	492	GLU	3.9
1	A	570	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	439	SER	3.8
1	B	464	PHE	3.8
1	A	569	VAL	3.7
1	A	528	ARG	3.7
1	A	499	LEU	3.7
1	B	101	GLY	3.6
1	A	555	ILE	3.5
1	A	515	LYS	3.4
1	B	562	GLN	3.3
1	A	457	SER	3.3
1	B	570	ALA	3.3
1	B	102	ALA	3.3
1	B	447	SER	3.2
1	A	488	GLU	3.2
1	B	433	ASP	3.1
1	A	447	SER	3.1
1	B	553	ARG	3.0
1	A	531	THR	3.0
1	B	461	THR	3.0
1	A	465	PRO	2.9
1	B	490	ASP	2.9
1	A	496	THR	2.9
1	B	440	GLN	2.9
1	A	445	LEU	2.9
1	A	493	ALA	2.9
1	B	509	TYR	2.8
1	A	464	PHE	2.8
1	B	525	ARG	2.8
1	B	456	THR	2.8
1	B	524	ILE	2.8
1	A	554	CYS	2.8
1	B	431	GLU	2.8
1	A	470	VAL	2.8
1	A	514	PHE	2.7
1	B	432	GLU	2.7
1	A	542	GLN	2.7
1	A	471	TYR	2.7
1	A	509	TYR	2.6
1	A	436	LYS	2.6
1	A	537	ASP	2.6
1	A	561	LEU	2.6
1	B	469	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	552	PRO	2.5
1	B	446	GLU	2.5
1	A	529	GLN	2.5
1	A	524	ILE	2.5
1	B	448	SER	2.4
1	A	434	LEU	2.4
1	A	440	GLN	2.4
1	B	419	ASN	2.4
1	A	458	TYR	2.4
1	A	495	SER	2.4
1	B	496	THR	2.4
1	A	534	SER	2.4
1	A	511	ARG	2.3
1	A	490	ASP	2.3
1	A	437	ALA	2.3
1	B	551	THR	2.3
1	B	472	LEU	2.3
1	B	468	TYR	2.2
1	A	473	GLU	2.2
1	B	462	SER	2.2
1	B	497	CYS	2.2
1	A	468	TYR	2.2
1	B	527	VAL	2.2
1	B	506	ASP	2.2
1	B	505	LEU	2.1
1	A	559	LYS	2.1
1	B	511	ARG	2.1
1	A	556	LYS	2.1
1	B	492	GLU	2.0
1	B	430	ASN	2.0
1	B	9	GLU	2.0
1	A	433	ASP	2.0
1	A	563	VAL	2.0
1	A	574	SER	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	SAL	B	601	10/10	0.91	0.15	3.01	19,26,29,31	0
2	SAL	A	601	10/10	0.95	0.12	0.59	18,24,26,28	0
3	AMP	A	602	23/23	0.96	0.12	-0.13	10,21,32,36	0
3	AMP	B	602	23/23	0.94	0.11	-0.28	12,22,30,36	0

6.5 Other polymers (i)

There are no such residues in this entry.