Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:22 PM GMT

PDB ID	:	1FCP
Title	:	FERRIC HYDROXAMATE UPTAKE RECEPTOR (FHUA) FROM E.COLI IN COMPLEX WITH BOUND FERRICHROME-IRON
Authors	:	Hofmann, E.; Ferguson, A.D.; Diederichs, K.; Welte, W.
Deposited on	:	1998-10-14
Resolution	:	2.70 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:

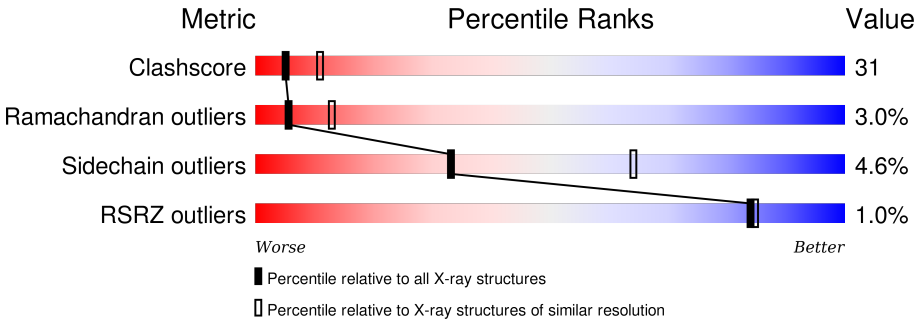
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.70 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	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	705	% 51% 44%

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	GAL	A	1007	X	-	-	-
2	GAL	A	1009	X	-	-	-
4	LIL	A	903	-	-	-	X
4	LIL	A	904	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	AAE	A	905	-	X	-	-
6	LIM	A	906	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 5832 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 PROTEIN (FERRIC HYDROXAMATE UPTAKE RECEPTOR).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	705	5512	3469	942	1087	4	10	0	0	0

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	406	SER	-	INSERTION	UNP P06971
A	407	HIS	-	INSERTION	UNP P06971
A	408	HIS	-	INSERTION	UNP P06971
A	409	HIS	-	INSERTION	UNP P06971
A	410	HIS	-	INSERTION	UNP P06971
A	411	HIS	-	INSERTION	UNP P06971
A	412	HIS	-	INSERTION	UNP P06971
A	413	GLY	-	INSERTION	UNP P06971
A	414	SER	-	INSERTION	UNP P06971
A	58	MSE	MET	MODIFIED RESIDUE	UNP P06971
A	125	MSE	MET	MODIFIED RESIDUE	UNP P06971
A	132	MSE	MET	MODIFIED RESIDUE	UNP P06971
A	151	MSE	MET	MODIFIED RESIDUE	UNP P06971
A	281	MSE	MET	MODIFIED RESIDUE	UNP P06971
A	381	MSE	MET	MODIFIED RESIDUE	UNP P06971
A	383	MSE	MET	MODIFIED RESIDUE	UNP P06971
A	559	MSE	MET	MODIFIED RESIDUE	UNP P06971
A	622	MSE	MET	MODIFIED RESIDUE	UNP P06971
A	680	MSE	MET	MODIFIED RESIDUE	UNP P06971

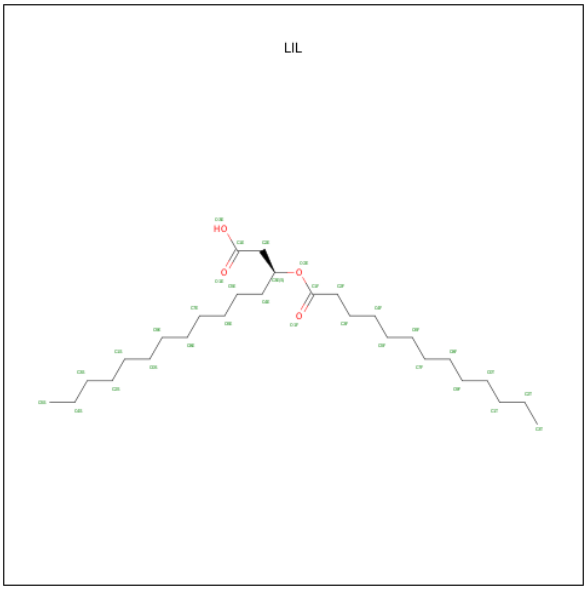
- Molecule 2 is a polymer of unknown type called SUGAR (9-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	9	124	60	2	59	3	0	0

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

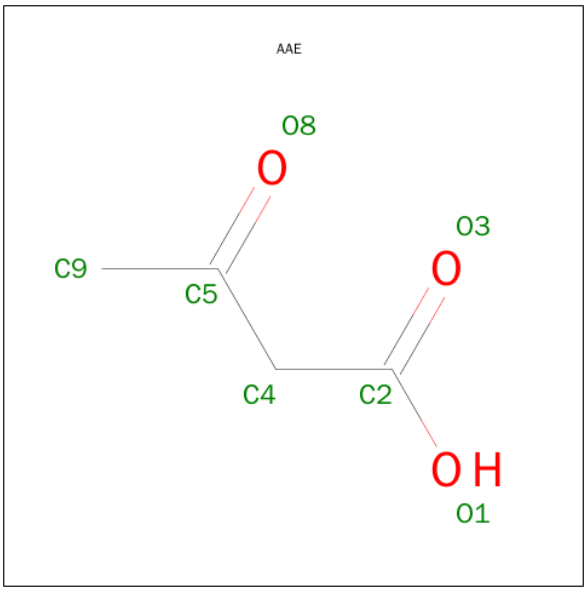
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Ni 2 2	0	0

- Molecule 4 is 2-TRIDECANOYLOXY-PENTADECANOIC ACID (three-letter code: LIL) (formula: $C_{28}H_{54}O_4$).



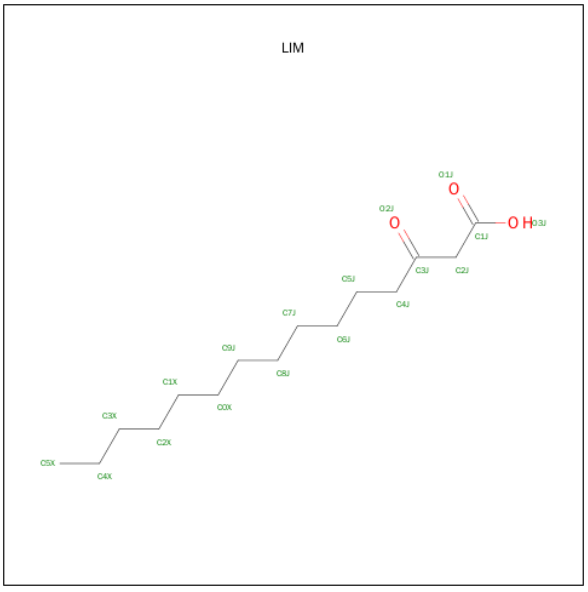
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 31 28 3	0	0
4	A	1	Total C O 31 28 3	0	0

- Molecule 5 is ACETOACETIC ACID (three-letter code: AAE) (formula: $C_4H_6O_3$).



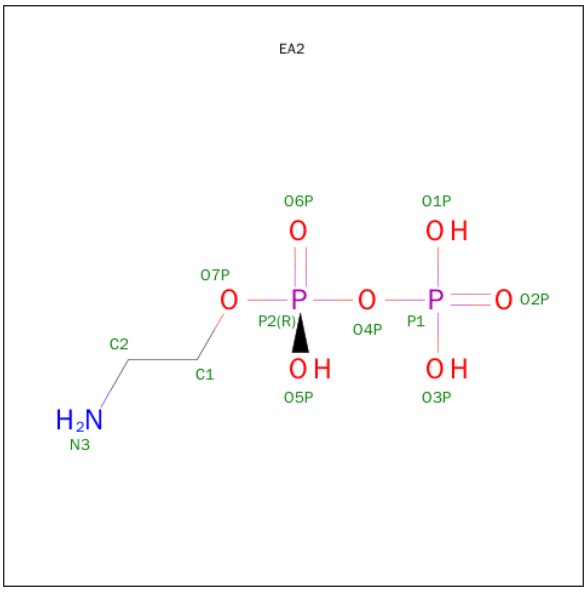
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 4 2	0	0

- Molecule 6 is 3-OXO-PENTADECANOIC ACID (three-letter code: LIM) (formula: $C_{15}H_{28}O_3$).



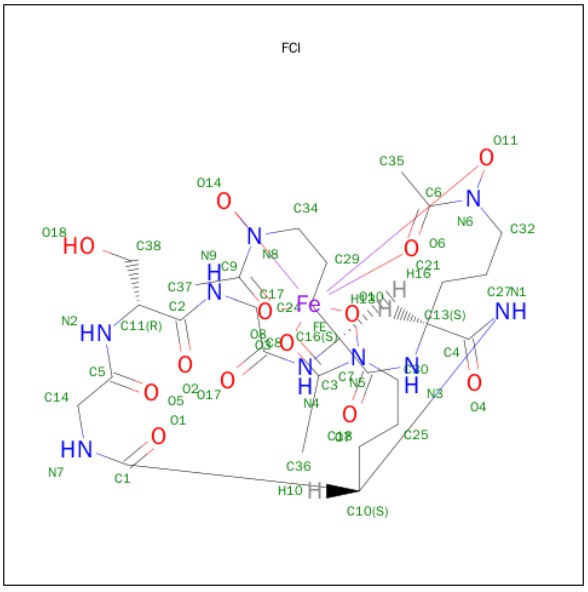
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 17 15 2	0	0

- Molecule 7 is AMINOETHANOLPYROPHOSPHATE (three-letter code: EA2) (formula: $C_2H_9NO_7P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			11	2	1	6	2		

- Molecule 8 is FERRICROCIN-IRON (three-letter code: FCI) (formula: $C_{28}H_{44}FeN_9O_{13}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	Fe	N	O	0	0
			46	24	1	9	12		

- Molecule 9 is water.

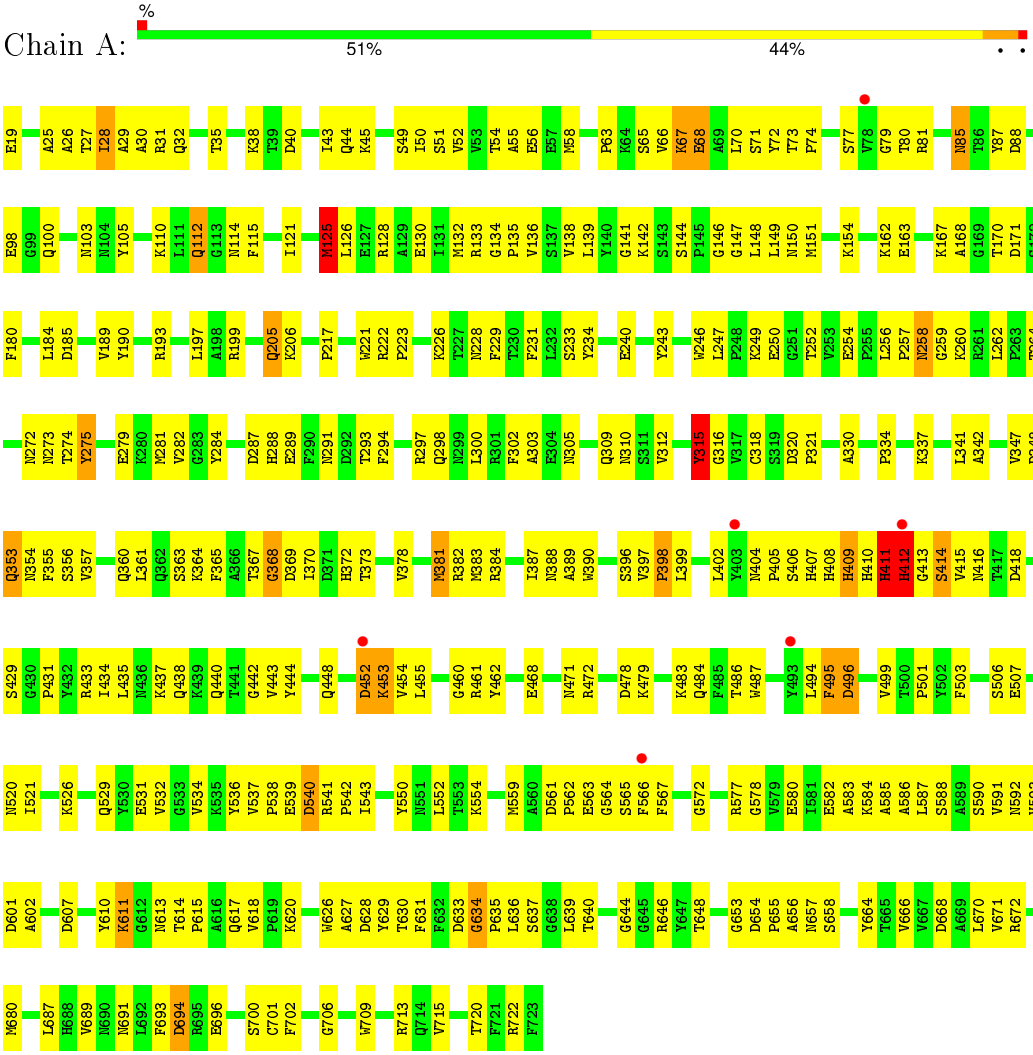
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	52	Total O 52 52	0	0

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: PROTEIN (FERRIC HYDROXAMATE UPTAKE RECEPTOR)

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	171.40Å 171.40Å 85.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.70 46.94 – 2.68	Depositor EDS
% Data completeness (in resolution range)	98.3 (40.00-2.70) 97.4 (46.94-2.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.44 (at 2.69Å)	Xtriage
Refinement program	CNS 0.4	Depositor
R, R_{free}	0.232 , 0.281 0.230 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	58.6	Xtriage
Anisotropy	0.596	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 55.6	EDS
Estimated twinning fraction	0.033 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 39633 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5832	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% 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: AAE, NI, KDO, GPH, LIL, LIM, GLC, GAL, GP4, FCI, GMH, EA2, GP1

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	0.45	2/5642 (0.0%)	0.71	8/7650 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	A	2	0
All	All	2	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	125	MSE	CG-SE	-5.73	1.75	1.95
1	A	680	MSE	CG-SE	-5.18	1.77	1.95

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	412	HIS	N-CA-C	15.24	152.14	111.00
1	A	412	HIS	CA-C-N	-9.20	97.79	116.20
1	A	409	HIS	N-CA-C	-7.00	92.10	111.00
1	A	411	HIS	N-CA-C	-6.74	92.82	111.00
1	A	412	HIS	CB-CA-C	-6.00	98.41	110.40
1	A	411	HIS	C-N-CA	5.20	134.71	121.70
1	A	315	TYR	C-N-CA	-5.05	111.69	122.30
1	A	315	TYR	N-CA-C	-5.01	97.48	111.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1007	GAL	C1
2	A	1009	GAL	C1

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	315	TYR	Sidechain
1	A	412	HIS	Mainchain

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	5512	0	5213	331	0
2	A	124	0	85	4	0
3	A	2	0	0	0	0
4	A	62	0	104	18	0
5	A	6	0	5	0	0
6	A	17	0	27	6	0
7	A	11	0	6	0	0
8	A	46	0	31	2	0
9	A	52	0	0	6	0
All	All	5832	0	5471	345	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 31.

All (345) 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:410:HIS:HA	1:A:412:HIS:ND1	1.69	1.06
1:A:121:ILE:HB	1:A:151:MSE:HE1	1.40	1.01
1:A:28:ILE:HD12	1:A:28:ILE:H	1.24	1.00
1:A:410:HIS:H	1:A:412:HIS:HB3	1.27	0.97
1:A:410:HIS:CA	1:A:412:HIS:ND1	2.29	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:MSE:HE2	1:A:136:VAL:HG12	1.49	0.95
1:A:134:GLY:CA	1:A:146:GLY:HA2	2.00	0.91
1:A:66:VAL:HG21	1:A:151:MSE:HE3	1.51	0.90
1:A:199:ARG:HD2	9:A:1054:HOH:O	1.75	0.86
1:A:341:LEU:HB2	1:A:402:LEU:HD11	1.58	0.84
1:A:453:LYS:HE2	1:A:453:LYS:N	1.93	0.83
1:A:274:THR:HG22	1:A:310:ASN:HB2	1.61	0.83
1:A:121:ILE:HB	1:A:151:MSE:CE	2.10	0.81
1:A:206:LYS:HD3	1:A:414:SER:H	1.45	0.81
1:A:468:GLU:HG3	1:A:479:LYS:HG2	1.62	0.81
1:A:125:MSE:HG3	1:A:234:TYR:HE1	1.46	0.80
1:A:206:LYS:CD	1:A:413:GLY:HA3	2.11	0.80
1:A:373:THR:HB	1:A:448:GLN:HB2	1.65	0.79
1:A:355:PHE:HB2	4:A:904:LIL:H2E1	1.64	0.79
1:A:453:LYS:HE2	1:A:453:LYS:H	1.48	0.78
1:A:228:ASN:HB3	1:A:287:ASP:OD1	1.83	0.78
1:A:309:GLN:HG2	1:A:348:ASP:HB3	1.66	0.77
1:A:410:HIS:HA	1:A:412:HIS:CE1	2.21	0.75
1:A:206:LYS:HG3	1:A:413:GLY:HA3	1.67	0.75
1:A:592:ASN:HB2	1:A:628:ASP:OD1	1.85	0.75
1:A:542:PRO:HG2	1:A:586:ALA:HB3	1.68	0.75
1:A:35:THR:HG21	1:A:150:ASN:HD22	1.50	0.74
1:A:71:SER:HB3	1:A:646:ARG:HD2	1.69	0.74
1:A:494:LEU:HD11	9:A:1047:HOH:O	1.87	0.74
1:A:410:HIS:N	1:A:412:HIS:HB3	2.02	0.74
1:A:31:ARG:HH12	1:A:539:GLU:HA	1.52	0.74
1:A:249:LYS:HG2	1:A:250:GLU:OE1	1.88	0.73
1:A:126:LEU:HD11	1:A:151:MSE:CE	2.18	0.73
2:A:1006:GLC:H61	2:A:1009:GAL:H5	1.69	0.73
1:A:35:THR:CG2	1:A:150:ASN:HD22	2.02	0.73
1:A:503:PHE:HB2	1:A:532:VAL:HG12	1.71	0.73
1:A:126:LEU:HD11	1:A:151:MSE:HE3	1.70	0.72
1:A:602:ALA:O	1:A:614:THR:HG22	1.91	0.71
1:A:330:ALA:HA	1:A:337:LYS:NZ	2.06	0.70
1:A:205:GLN:HG3	1:A:243:TYR:CG	2.26	0.70
1:A:93:ARG:HD3	1:A:133:ARG:HG2	1.73	0.70
1:A:409:HIS:O	1:A:410:HIS:HB2	1.90	0.70
1:A:444:TYR:HB3	1:A:461:ARG:HB2	1.74	0.69
1:A:206:LYS:CG	1:A:413:GLY:HA3	2.22	0.69
4:A:903:LIL:H8E1	4:A:904:LIL:H8E1	1.74	0.68
1:A:384:ARG:NH1	1:A:437:LYS:HE2	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:VAL:HG22	1:A:416:ASN:N	2.08	0.68
1:A:28:ILE:H	1:A:28:ILE:CD1	2.02	0.67
1:A:390:TRP:CZ3	1:A:431:PRO:HB3	2.28	0.67
1:A:407:HIS:O	1:A:409:HIS:O	2.13	0.67
1:A:154:LYS:HD3	1:A:193:ARG:NH2	2.11	0.66
1:A:134:GLY:HA2	1:A:146:GLY:HA2	1.78	0.66
1:A:217:PRO:HD2	1:A:233:SER:OG	1.95	0.66
1:A:98:GLU:OE2	1:A:554:LYS:NZ	2.27	0.66
1:A:167:LYS:HB2	1:A:175:GLN:HB3	1.78	0.65
1:A:415:VAL:HG22	1:A:416:ASN:H	1.62	0.65
1:A:410:HIS:H	1:A:412:HIS:CB	2.05	0.65
1:A:713:ARG:HG2	1:A:713:ARG:HH11	1.63	0.64
1:A:134:GLY:C	1:A:146:GLY:HA2	2.18	0.64
1:A:297:ARG:HG3	1:A:360:GLN:HG3	1.80	0.63
1:A:125:MSE:HG3	1:A:234:TYR:CE1	2.32	0.63
1:A:126:LEU:HD21	1:A:151:MSE:HE2	1.79	0.63
1:A:19:GLU:O	1:A:32:GLN:HG3	1.97	0.63
2:A:1006:GLC:H61	2:A:1009:GAL:C5	2.29	0.63
1:A:282:VAL:HG21	4:A:903:LIL:H9E1	1.81	0.63
1:A:352:LEU:HB2	1:A:384:ARG:O	1.99	0.63
1:A:590:SER:HB2	1:A:630:THR:O	2.00	0.62
1:A:189:VAL:HG13	1:A:190:TYR:CD2	2.35	0.62
1:A:397:VAL:HG23	1:A:398:PRO:HD2	1.82	0.62
1:A:381:MSE:HE1	1:A:383:MSE:HB2	1.82	0.62
4:A:903:LIL:H2E2	4:A:904:LIL:H4E2	1.82	0.62
1:A:67:LYS:HB2	1:A:67:LYS:HZ2	1.64	0.62
1:A:626:TRP:CH2	1:A:628:ASP:HB3	2.34	0.61
1:A:666:VAL:HG13	1:A:691:ASN:HA	1.81	0.61
1:A:58:MSE:O	1:A:63:PRO:HD2	2.00	0.61
1:A:543:ILE:HG22	1:A:585:ALA:HB1	1.82	0.61
1:A:105:TYR:O	1:A:150:ASN:HA	2.01	0.60
1:A:671:VAL:CG2	1:A:687:LEU:HB3	2.31	0.60
1:A:221:TRP:CE2	1:A:223:PRO:HG3	2.37	0.60
1:A:297:ARG:HD2	1:A:360:GLN:NE2	2.17	0.59
1:A:559:MSE:HE2	1:A:572:GLY:N	2.17	0.59
1:A:565:SER:C	1:A:567:PHE:H	2.05	0.59
1:A:162:LYS:HA	1:A:180:PHE:HD1	1.66	0.59
1:A:66:VAL:HG21	1:A:151:MSE:CE	2.29	0.59
1:A:28:ILE:HG13	1:A:56:GLU:OE1	2.02	0.59
1:A:93:ARG:HG3	1:A:550:TYR:OH	2.02	0.59
1:A:231:PHE:CZ	4:A:903:LIL:H4S2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:GLY:HA2	1:A:487:TRP:HA	1.84	0.59
1:A:565:SER:O	1:A:567:PHE:N	2.32	0.59
1:A:71:SER:HB3	1:A:646:ARG:CD	2.31	0.59
1:A:353:GLN:OE1	1:A:384:ARG:HD3	2.03	0.58
1:A:282:VAL:HG11	4:A:903:LIL:H7F2	1.85	0.58
1:A:390:TRP:HE1	1:A:429:SER:CB	2.15	0.58
1:A:138:VAL:HG13	1:A:139:LEU:HG	1.86	0.58
1:A:133:ARG:HD2	1:A:580:GLU:OE1	2.03	0.58
1:A:501:PRO:HA	1:A:534:VAL:HG12	1.84	0.58
1:A:134:GLY:N	1:A:146:GLY:HA2	2.17	0.58
4:A:903:LIL:H9E2	4:A:904:LIL:H0S1	1.85	0.58
1:A:197:LEU:HD12	1:A:197:LEU:C	2.24	0.58
1:A:135:PRO:HB2	1:A:506:SER:OG	2.04	0.58
1:A:577:ARG:HH11	1:A:577:ARG:HG3	1.68	0.57
1:A:384:ARG:HH12	1:A:437:LYS:HE2	1.68	0.57
1:A:74:PRO:HG3	1:A:582:GLU:HB2	1.87	0.57
1:A:79:GLY:C	1:A:81:ARG:H	2.08	0.57
1:A:434:ILE:HD13	1:A:471:ASN:HA	1.87	0.57
1:A:689:VAL:HG22	1:A:715:VAL:HG22	1.86	0.57
1:A:49:SER:C	1:A:50:ILE:HD12	2.25	0.57
1:A:316:GLY:O	1:A:341:LEU:HD12	2.05	0.57
1:A:162:LYS:HA	1:A:180:PHE:CD1	2.40	0.56
1:A:206:LYS:HG3	1:A:413:GLY:CA	2.35	0.56
1:A:294:PHE:HE1	1:A:363:SER:HG	1.53	0.56
1:A:105:TYR:CE2	1:A:110:LYS:HB2	2.39	0.56
1:A:611:LYS:C	1:A:613:ASN:H	2.08	0.56
1:A:388:ASN:HD22	1:A:433:ARG:HG2	1.70	0.56
1:A:350:GLU:HG2	1:A:387:ILE:HG12	1.87	0.56
1:A:25:ALA:O	1:A:26:ALA:HB3	2.05	0.56
1:A:529:GLN:HB2	1:A:552:LEU:HD13	1.88	0.56
1:A:370:ILE:HG22	1:A:372:HIS:CD2	2.40	0.56
4:A:904:LIL:H9F1	6:A:906:LIM:H5X2	1.87	0.56
1:A:615:PRO:O	1:A:618:VAL:HG12	2.06	0.55
1:A:185:ASP:OD2	1:A:189:VAL:HG12	2.07	0.55
1:A:67:LYS:HE3	1:A:87:TYR:O	2.07	0.55
1:A:607:ASP:HB3	1:A:610:TYR:O	2.06	0.55
1:A:148:LEU:HD23	1:A:148:LEU:C	2.27	0.55
1:A:249:LYS:HE2	1:A:254:GLU:OE1	2.07	0.55
1:A:258:ASN:HD22	1:A:260:LYS:HD2	1.72	0.55
1:A:247:LEU:HD21	1:A:268:GLU:HG3	1.88	0.55
1:A:93:ARG:NH1	1:A:580:GLU:OE1	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:ASP:OD2	1:A:658:SER:HB3	2.07	0.55
1:A:52:VAL:HG22	1:A:130:GLU:HG2	1.88	0.54
1:A:93:ARG:HH11	1:A:580:GLU:CD	2.10	0.54
1:A:19:GLU:OE2	1:A:30:ALA:HA	2.06	0.54
1:A:390:TRP:CD2	1:A:424:LYS:HG3	2.42	0.54
1:A:672:ARG:HD2	9:A:1028:HOH:O	2.06	0.54
1:A:300:LEU:C	1:A:300:LEU:HD23	2.28	0.54
1:A:300:LEU:CG	1:A:357:VAL:HG12	2.38	0.54
1:A:590:SER:O	1:A:629:TYR:HA	2.08	0.54
1:A:531:GLU:HG3	1:A:550:TYR:HB3	1.90	0.54
1:A:341:LEU:CB	1:A:402:LEU:HD11	2.35	0.53
1:A:297:ARG:CG	1:A:360:GLN:HG3	2.38	0.53
1:A:310:ASN:ND2	1:A:347:VAL:HG13	2.24	0.53
1:A:408:HIS:O	1:A:411:HIS:HB2	2.08	0.53
1:A:66:VAL:CG2	1:A:151:MSE:HE3	2.31	0.53
1:A:51:SER:OG	1:A:133:ARG:NH2	2.39	0.53
1:A:189:VAL:HG23	1:A:222:ARG:O	2.07	0.53
1:A:49:SER:O	1:A:50:ILE:HD12	2.08	0.53
1:A:352:LEU:C	1:A:352:LEU:HD12	2.28	0.52
1:A:368:GLY:O	1:A:369:ASP:HB2	2.08	0.52
1:A:646:ARG:NH1	1:A:668:ASP:OD2	2.42	0.52
1:A:288:HIS:ND1	1:A:289:GLU:N	2.57	0.52
1:A:355:PHE:CB	4:A:904:LIL:H2E1	2.37	0.52
1:A:484:GLN:OE1	1:A:526:LYS:HE2	2.08	0.52
1:A:409:HIS:O	1:A:410:HIS:CB	2.54	0.52
1:A:264:THR:HA	1:A:709:TRP:CD1	2.45	0.52
1:A:637:SER:HB3	1:A:677:ARG:HH21	1.75	0.52
4:A:904:LIL:H7F1	6:A:906:LIM:C0X	2.40	0.52
1:A:264:THR:HG21	1:A:696:GLU:HG2	1.92	0.51
1:A:294:PHE:CD1	1:A:361:LEU:HD11	2.45	0.51
1:A:279:GLU:HA	1:A:305:ASN:OD1	2.11	0.51
1:A:631:PHE:HB2	1:A:636:LEU:O	2.10	0.51
1:A:298:GLN:HE22	6:A:906:LIM:H3X1	1.73	0.51
1:A:205:GLN:HG3	1:A:243:TYR:HB2	1.92	0.51
1:A:103:ASN:ND2	1:A:147:GLY:O	2.44	0.51
1:A:170:THR:HG22	1:A:171:ASP:N	2.27	0.50
1:A:540:ASP:OD2	1:A:541:ARG:HG3	2.11	0.50
1:A:407:HIS:C	1:A:409:HIS:O	2.49	0.50
1:A:462:TYR:OH	1:A:483:LYS:HB3	2.12	0.50
1:A:542:PRO:CG	1:A:586:ALA:HB3	2.40	0.50
1:A:135:PRO:HB3	1:A:507:GLU:C	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:PHE:HZ	4:A:904:LIL:H5S2	1.77	0.50
1:A:67:LYS:HD3	9:A:1043:HOH:O	2.11	0.50
1:A:701:CYS:HA	1:A:706:GLY:O	2.11	0.50
1:A:410:HIS:N	1:A:412:HIS:ND1	2.60	0.50
1:A:281:MSE:HB3	1:A:303:ALA:HB2	1.94	0.50
1:A:205:GLN:HG3	1:A:243:TYR:CB	2.41	0.50
1:A:670:LEU:HD12	1:A:671:VAL:N	2.26	0.50
1:A:413:GLY:O	1:A:414:SER:HB2	2.11	0.50
1:A:142:LYS:NZ	1:A:438:GLN:OE1	2.45	0.50
1:A:671:VAL:HG22	1:A:687:LEU:HB3	1.93	0.49
1:A:79:GLY:C	1:A:81:ARG:N	2.65	0.49
1:A:168:ALA:HA	1:A:173:LEU:O	2.12	0.49
1:A:676:ALA:C	1:A:678:VAL:H	2.15	0.49
1:A:80:THR:HG22	1:A:80:THR:O	2.12	0.49
1:A:588:SER:HB3	1:A:591:VAL:HB	1.94	0.49
1:A:302:PHE:HZ	4:A:903:LIL:H2E1	1.77	0.49
1:A:67:LYS:HG3	1:A:88:ASP:HA	1.93	0.49
1:A:529:GLN:HB2	1:A:552:LEU:CD1	2.42	0.49
1:A:32:GLN:O	1:A:128:ARG:NH2	2.44	0.49
1:A:383:MSE:HE1	1:A:438:GLN:NE2	2.27	0.49
1:A:671:VAL:HG23	1:A:671:VAL:O	2.12	0.49
1:A:257:PRO:C	1:A:259:GLY:H	2.16	0.49
1:A:65:SER:OG	1:A:67:LYS:HB2	2.13	0.49
1:A:130:GLU:O	1:A:149:LEU:HD12	2.12	0.49
1:A:302:PHE:CZ	4:A:903:LIL:H2E1	2.47	0.48
1:A:390:TRP:CE2	1:A:424:LYS:HB2	2.48	0.48
1:A:610:TYR:O	1:A:611:LYS:HB2	2.13	0.48
1:A:38:LYS:HG3	1:A:139:LEU:HD22	1.95	0.48
1:A:294:PHE:HD1	1:A:361:LEU:HD11	1.78	0.48
1:A:265:ASP:CG	1:A:412:HIS:HD2	2.16	0.48
1:A:72:TYR:CE2	1:A:626:TRP:HB2	2.48	0.48
1:A:626:TRP:CD1	1:A:644:GLY:HA3	2.48	0.48
1:A:265:ASP:OD1	1:A:412:HIS:CD2	2.67	0.48
1:A:258:ASN:ND2	1:A:260:LYS:HD2	2.28	0.48
1:A:45:LYS:HB3	1:A:455:LEU:CD2	2.44	0.48
1:A:282:VAL:HG21	4:A:903:LIL:C9E	2.43	0.48
1:A:93:ARG:HG3	1:A:550:TYR:CZ	2.48	0.48
1:A:415:VAL:CG2	1:A:416:ASN:H	2.26	0.48
1:A:256:LEU:HD11	1:A:402:LEU:HB3	1.96	0.48
1:A:594:VAL:O	1:A:626:TRP:N	2.44	0.48
1:A:67:LYS:HB2	1:A:67:LYS:NZ	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:610:TYR:CZ	1:A:655:PRO:HB2	2.49	0.48
1:A:252:THR:HG22	1:A:709:TRP:CE2	2.48	0.48
1:A:406:SER:O	1:A:410:HIS:HD2	1.97	0.48
1:A:184:LEU:HD12	1:A:190:TYR:HB3	1.95	0.48
1:A:284:TYR:OH	6:A:906:LIM:H5X3	2.14	0.48
1:A:415:VAL:CG2	1:A:416:ASN:N	2.75	0.48
1:A:578:GLY:HA3	1:A:599:TYR:O	2.13	0.48
1:A:297:ARG:HG3	1:A:360:GLN:CG	2.44	0.48
1:A:478:ASP:HB3	1:A:521:ILE:HD11	1.96	0.48
1:A:134:GLY:H	1:A:146:GLY:HA2	1.78	0.47
1:A:38:LYS:HE3	1:A:139:LEU:O	2.14	0.47
1:A:114:ASN:HB2	9:A:1023:HOH:O	2.14	0.47
1:A:27:THR:HG22	1:A:28:ILE:N	2.30	0.47
1:A:330:ALA:HA	1:A:337:LYS:HZ1	1.77	0.47
1:A:262:LEU:HD13	1:A:266:PHE:CD2	2.48	0.47
4:A:904:LIL:H2F2	6:A:906:LIM:O1J	2.14	0.47
1:A:593:VAL:HG12	1:A:627:ALA:HB2	1.96	0.47
1:A:246:TRP:HB3	1:A:706:GLY:HA2	1.94	0.47
1:A:367:THR:HG22	1:A:367:THR:O	2.15	0.47
1:A:342:ALA:HA	1:A:399:LEU:HD22	1.96	0.47
1:A:31:ARG:NH2	1:A:541:ARG:O	2.48	0.47
1:A:615:PRO:HG2	1:A:618:VAL:HG11	1.97	0.47
1:A:678:VAL:O	1:A:678:VAL:HG12	2.14	0.47
1:A:636:LEU:HD22	1:A:639:LEU:HD22	1.97	0.47
1:A:320:ASP:OD1	1:A:321:PRO:HD2	2.14	0.47
1:A:565:SER:C	1:A:567:PHE:N	2.68	0.46
1:A:356:SER:HB3	9:A:1051:HOH:O	2.14	0.46
1:A:390:TRP:HE1	1:A:429:SER:HB2	1.80	0.46
1:A:206:LYS:HD3	1:A:413:GLY:HA3	1.93	0.46
1:A:495:PHE:HB2	1:A:499:VAL:O	2.16	0.46
1:A:112:GLN:HE21	1:A:112:GLN:CA	2.28	0.46
1:A:347:VAL:O	1:A:389:ALA:HB1	2.16	0.46
1:A:577:ARG:O	1:A:601:ASP:HB3	2.16	0.46
1:A:77:SER:OG	1:A:91:ILE:HB	2.15	0.46
1:A:518:ASP:OD2	1:A:520:ASN:HB2	2.16	0.46
1:A:154:LYS:HD3	1:A:193:ARG:CZ	2.46	0.46
1:A:297:ARG:HD2	1:A:360:GLN:HE21	1.81	0.46
1:A:126:LEU:HD11	1:A:151:MSE:HE2	1.97	0.46
1:A:199:ARG:HG3	1:A:199:ARG:HH11	1.80	0.46
4:A:903:LIL:H3E1	4:A:903:LIL:H2F2	1.72	0.46
1:A:67:LYS:HZ1	1:A:85:ASN:ND2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:LEU:CB	1:A:357:VAL:HG12	2.46	0.46
1:A:114:ASN:OD1	1:A:387:ILE:HD11	2.16	0.45
1:A:536:TYR:CD2	1:A:538:PRO:HD3	2.51	0.45
1:A:390:TRP:CE2	1:A:424:LYS:HG3	2.51	0.45
1:A:402:LEU:C	1:A:405:PRO:HD2	2.36	0.45
1:A:402:LEU:O	1:A:405:PRO:HD2	2.17	0.45
1:A:105:TYR:CZ	1:A:110:LYS:HB2	2.52	0.45
1:A:265:ASP:CG	1:A:412:HIS:CD2	2.91	0.45
1:A:265:ASP:OD2	1:A:413:GLY:HA2	2.17	0.45
1:A:599:TYR:OH	1:A:620:LYS:NZ	2.50	0.45
1:A:617:GLN:HG2	1:A:700:SER:HB2	1.99	0.45
1:A:185:ASP:CG	1:A:189:VAL:HG12	2.38	0.44
1:A:240:GLU:HA	1:A:275:TYR:O	2.17	0.44
2:A:1006:GLC:C6	2:A:1009:GAL:C5	2.95	0.44
1:A:197:LEU:O	1:A:197:LEU:HD12	2.18	0.44
1:A:722:ARG:HH11	1:A:722:ARG:HG3	1.82	0.44
1:A:65:SER:HB3	1:A:85:ASN:OD1	2.16	0.44
1:A:258:ASN:HD22	1:A:260:LYS:CD	2.31	0.44
1:A:100:GLN:HG3	8:A:750:FCI:C9	2.48	0.44
1:A:691:ASN:HB3	1:A:713:ARG:HA	2.00	0.44
1:A:565:SER:O	1:A:566:PHE:HB2	2.18	0.44
1:A:653:GLY:O	1:A:654:ASP:HB3	2.17	0.44
1:A:44:GLN:HG2	1:A:45:LYS:N	2.32	0.44
1:A:519:GLY:O	1:A:520:ASN:ND2	2.51	0.44
1:A:406:SER:O	1:A:410:HIS:CD2	2.70	0.44
1:A:592:ASN:O	1:A:627:ALA:HA	2.18	0.44
1:A:713:ARG:NH1	1:A:713:ARG:HG2	2.32	0.44
1:A:300:LEU:HG	1:A:357:VAL:HG12	1.99	0.44
1:A:634:GLY:HA3	1:A:635:PRO:HD2	1.90	0.44
1:A:378:VAL:HA	1:A:442:GLY:O	2.19	0.43
1:A:562:PRO:HB2	1:A:563:GLU:OE1	2.18	0.43
1:A:309:GLN:O	1:A:347:VAL:HA	2.17	0.43
4:A:904:LIL:H1T1	6:A:906:LIM:H5X1	1.99	0.43
1:A:273:ASN:HD21	1:A:312:VAL:H	1.65	0.43
1:A:141:GLY:HA3	1:A:440:GLN:NE2	2.33	0.43
4:A:903:LIL:H5E2	4:A:903:LIL:H4F1	1.99	0.43
1:A:352:LEU:O	1:A:352:LEU:HD12	2.19	0.43
1:A:93:ARG:HD2	1:A:580:GLU:OE2	2.19	0.43
1:A:559:MSE:SE	1:A:607:ASP:HA	2.68	0.43
1:A:676:ALA:O	1:A:678:VAL:N	2.47	0.43
1:A:206:LYS:HD2	1:A:413:GLY:HA3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:ASN:ND2	1:A:433:ARG:CD	2.82	0.43
1:A:226:LYS:HB3	1:A:289:GLU:HB3	1.99	0.43
1:A:702:PHE:CE2	1:A:706:GLY:HA3	2.54	0.43
1:A:144:SER:HA	1:A:510:GLU:OE1	2.18	0.43
1:A:364:LYS:CD	1:A:373:THR:HG23	2.48	0.43
1:A:611:LYS:C	1:A:613:ASN:N	2.72	0.43
2:A:1005:GPH:O2	2:A:1006:GLC:H5	2.19	0.43
1:A:443:VAL:O	1:A:443:VAL:HG23	2.18	0.43
1:A:303:ALA:O	1:A:353:GLN:HA	2.19	0.42
1:A:410:HIS:H	1:A:412:HIS:CG	2.37	0.42
1:A:68:GLU:C	1:A:70:LEU:H	2.23	0.42
1:A:452:ASP:C	1:A:454:VAL:H	2.22	0.42
1:A:637:SER:HB3	1:A:677:ARG:HE	1.84	0.42
1:A:291:ASN:OD1	1:A:293:THR:HG22	2.19	0.42
1:A:27:THR:C	1:A:29:ALA:H	2.21	0.42
1:A:300:LEU:HB2	1:A:357:VAL:HG12	2.01	0.42
1:A:388:ASN:ND2	1:A:433:ARG:HD3	2.34	0.42
1:A:640:THR:HB	1:A:672:ARG:HB3	2.02	0.42
1:A:536:TYR:CZ	1:A:538:PRO:HB3	2.54	0.42
1:A:648:THR:HB	1:A:664:TYR:CE1	2.54	0.42
1:A:396:SER:HA	1:A:428:ASN:HB2	2.02	0.42
1:A:656:ALA:O	1:A:657:ASN:HB2	2.19	0.42
1:A:424:LYS:HD3	1:A:424:LYS:N	2.35	0.42
8:A:750:FCI:H212	8:A:750:FCI:O11	2.19	0.42
1:A:68:GLU:C	1:A:70:LEU:N	2.72	0.42
1:A:365:PHE:HE1	1:A:372:HIS:ND1	2.18	0.41
1:A:382:ARG:HG3	1:A:382:ARG:O	2.20	0.41
1:A:453:LYS:HE2	1:A:453:LYS:CA	2.50	0.41
1:A:31:ARG:NH1	1:A:539:GLU:HA	2.27	0.41
1:A:693:PHE:O	1:A:694:ASP:C	2.59	0.41
1:A:586:ALA:HA	1:A:592:ASN:HD22	1.85	0.41
1:A:350:GLU:CG	1:A:387:ILE:HG12	2.50	0.41
1:A:163:GLU:HB2	1:A:722:ARG:HD3	2.02	0.41
1:A:43:ILE:HG13	1:A:537:VAL:HG21	2.02	0.41
1:A:618:VAL:O	1:A:618:VAL:HG13	2.20	0.41
1:A:561:ASP:OD1	1:A:562:PRO:HD2	2.21	0.41
1:A:79:GLY:O	1:A:81:ARG:N	2.54	0.41
1:A:148:LEU:HD23	1:A:149:LEU:N	2.36	0.41
1:A:272:ASN:HB3	1:A:418:ASP:OD1	2.20	0.41
1:A:583:ALA:O	1:A:594:VAL:HA	2.21	0.41
1:A:577:ARG:HG3	1:A:577:ARG:NH1	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:ILE:HG22	1:A:435:LEU:N	2.35	0.41
1:A:126:LEU:HD13	1:A:151:MSE:HB3	2.03	0.41
1:A:543:ILE:CG2	1:A:585:ALA:HB1	2.48	0.41
1:A:27:THR:C	1:A:29:ALA:N	2.74	0.40
1:A:494:LEU:O	1:A:495:PHE:O	2.40	0.40
1:A:390:TRP:NE1	1:A:424:LYS:HB2	2.37	0.40
1:A:378:VAL:HG12	1:A:443:VAL:HG12	2.03	0.40
1:A:526:LYS:O	1:A:554:LYS:HA	2.21	0.40
1:A:55:ALA:HA	1:A:58:MSE:HE3	2.02	0.40
1:A:300:LEU:HG	1:A:357:VAL:CG1	2.51	0.40
1:A:584:LYS:HG2	1:A:594:VAL:HG22	2.03	0.40
1:A:390:TRP:NE1	1:A:429:SER:HB2	2.36	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	703/705 (100%)	624 (89%)	58 (8%)	21 (3%)	5 13

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	495	PHE
1	A	633	ASP
1	A	634	GLY
1	A	368	GLY
1	A	414	SER
1	A	452	ASP
1	A	564	GLY
1	A	611	LYS
1	A	677	ARG

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Mol	Chain	Res	Type
1	A	694	ASP
1	A	258	ASN
1	A	334	PRO
1	A	412	HIS
1	A	587	LEU
1	A	678	VAL
1	A	40	ASP
1	A	423	ALA
1	A	472	ARG
1	A	496	ASP
1	A	318	CYS
1	A	398	PRO

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	585/575 (102%)	558 (95%)	27 (5%)	33 64

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ILE
1	A	54	THR
1	A	67	LYS
1	A	68	GLU
1	A	73	THR
1	A	85	ASN
1	A	93	ARG
1	A	112	GLN
1	A	115	PHE
1	A	125	MSE
1	A	205	GLN
1	A	268	GLU
1	A	275	TYR
1	A	315	TYR

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Mol	Chain	Res	Type
1	A	352	LEU
1	A	353	GLN
1	A	354	ASN
1	A	381	MSE
1	A	404	ASN
1	A	411	HIS
1	A	424	LYS
1	A	428	ASN
1	A	453	LYS
1	A	486	THR
1	A	496	ASP
1	A	540	ASP
1	A	720	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	85	ASN
1	A	102	GLN
1	A	112	GLN
1	A	150	ASN
1	A	202	ASN
1	A	205	GLN
1	A	310	ASN
1	A	328	GLN
1	A	354	ASN
1	A	360	GLN
1	A	388	ASN
1	A	404	ASN
1	A	410	HIS
1	A	428	ASN
1	A	520	ASN
1	A	592	ASN

5.3.3 RNA

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)

9 carbohydrates 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	KDO	A	1002	2	12,15,16	0.75	0	12,21,24	0.92	1 (8%)
2	KDO	A	1003	2	12,15,16	0.38	0	12,21,24	0.82	0
2	GMH	A	1004	2,7	13,13,14	0.86	0	17,18,20	1.28	2 (11%)
2	GPH	A	1005	3,2	17,17,18	1.28	3 (17%)	22,25,27	1.40	3 (13%)
2	GLC	A	1006	2	11,11,12	0.68	0	14,15,17	1.31	2 (14%)
2	GAL	A	1007	2	11,11,12	0.64	0	14,15,17	1.18	2 (14%)
2	GAL	A	1009	2	11,11,12	0.65	0	14,15,17	0.90	1 (7%)
2	GP4	A	901	2,4	15,15,16	1.31	2 (13%)	18,22,24	1.93	3 (16%)
2	GP1	A	902	3,2,5,6	15,16,16	1.21	1 (6%)	20,24,24	0.73	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
2	KDO	A	1002	2	-	0/6/26/30	0/1/1/1
2	KDO	A	1003	2	-	0/6/26/30	0/1/1/1
2	GMH	A	1004	2,7	-	0/6/23/26	0/1/1/1
2	GPH	A	1005	3,2	-	0/11/28/31	0/1/1/1
2	GLC	A	1006	2	-	0/2/19/22	0/1/1/1
2	GAL	A	1007	2	1/1/4/5	0/2/19/22	0/1/1/1
2	GAL	A	1009	2	1/1/4/5	0/2/19/22	0/1/1/1
2	GP4	A	901	2,4	-	0/7/24/27	0/1/1/1
2	GP1	A	902	3,2,5,6	-	0/6/27/27	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	GP4	P4A-O4A	-3.29	1.50	1.60
2	A	902	GP1	P4B-O1B	-3.09	1.50	1.60
2	A	1005	GPH	P1-O4	-2.34	1.52	1.60
2	A	1005	GPH	C5-C4	2.07	1.56	1.52
2	A	1005	GPH	O5-C5	2.39	1.46	1.43
2	A	901	GP4	C1A-C2A	2.68	1.55	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	901	GP4	P4A-O4A-C4A	-3.80	112.45	121.56
2	A	1005	GPH	P1-O4-C4	-3.69	112.72	121.56
2	A	1002	KDO	C4-C5-C6	-2.41	105.56	110.56
2	A	1006	GLC	C1-C2-C3	-2.29	106.83	109.54
2	A	1005	GPH	C1-O5-C5	2.08	114.89	111.52
2	A	1009	GAL	C1-O5-C5	2.25	115.11	112.25
2	A	1007	GAL	C1-C2-C3	2.27	112.23	109.54
2	A	1006	GLC	C1-O5-C5	2.57	115.51	112.25
2	A	1004	GMH	O3-C3-C2	2.96	115.34	110.00
2	A	1005	GPH	C1-C2-C3	2.97	113.05	109.54
2	A	1004	GMH	O5-C5-C6	3.31	110.47	106.04
2	A	1007	GAL	C1-O5-C5	3.61	116.83	112.25
2	A	901	GP4	C1A-O6A-C5A	3.64	116.87	112.25
2	A	901	GP4	C1A-C2A-C3A	5.43	118.05	109.27

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1007	GAL	C1
2	A	1009	GAL	C1

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1005	GPH	1	0
2	A	1006	GLC	4	0
2	A	1009	GAL	3	0

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
7	EA2	A	1008	2	5,10,11	1.30	1 (20%)	6,13,16	1.22	1 (16%)
8	FCI	A	750	-	42,51,56	0.41	0	51,78,87	0.40	0
4	LIL	A	903	2	30,30,31	0.74	1 (3%)	30,31,33	0.98	1 (3%)
4	LIL	A	904	2	30,30,31	20.56	4 (13%)	30,31,33	9.08	5 (16%)
5	AAE	A	905	2	5,5,6	3.30	2 (40%)	5,5,7	3.79	4 (80%)
6	LIM	A	906	2	16,16,17	3.04	1 (6%)	13,16,18	2.13	2 (15%)

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
7	EA2	A	1008	2	-	0/8/10/11	0/0/0/0
8	FCI	A	750	-	-	0/57/102/116	0/0/6/6
4	LIL	A	903	2	-	2/31/31/32	0/0/0/0
4	LIL	A	904	2	-	1/31/31/32	0/0/0/0
5	AAE	A	905	2	-	0/3/3/4	0/0/0/0
6	LIM	A	906	2	-	0/14/15/16	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	905	AAE	O1-C2	-3.34	1.24	1.42
7	A	1008	EA2	P2-O7P	-2.03	1.49	1.59
4	A	904	LIL	O2E-C1F	3.30	1.44	1.34
4	A	903	LIL	O2E-C1F	3.66	1.45	1.34
5	A	905	AAE	O8-C5	6.29	1.43	1.21
6	A	906	LIM	O2J-C3J	12.01	1.43	1.21
4	A	904	LIL	C2E-C3E	27.62	2.54	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	904	LIL	O1F-C1F	67.38	3.23	1.22
4	A	904	LIL	C2E-C1E	85.83	4.24	1.49

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	904	LIL	C3E-C2E-C1E	-36.28	33.33	111.81
4	A	904	LIL	O2E-C1F-O1F	-29.48	44.55	123.67
4	A	904	LIL	O1E-C1E-C2E	-11.97	81.55	125.24
4	A	904	LIL	O2E-C3E-C2E	-11.28	61.56	108.28
6	A	906	LIM	O2J-C3J-C2J	-6.53	109.68	120.82
5	A	905	AAE	O8-C5-C4	-6.25	109.64	121.46
5	A	905	AAE	O8-C5-C9	-4.80	109.47	121.31
4	A	903	LIL	O2E-C1F-O1F	-3.80	113.46	123.67
6	A	906	LIM	O2J-C3J-C4J	-3.55	109.93	121.16
5	A	905	AAE	C9-C5-C4	-2.24	110.83	117.19
4	A	904	LIL	O1F-C1F-C2F	-2.03	115.61	123.72
7	A	1008	EA2	O4P-P2-O7P	2.08	108.45	102.94
5	A	905	AAE	O1-C2-C4	2.17	120.33	111.02

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	903	LIL	C3E-O2E-C1F-C2F
4	A	904	LIL	C1F-O2E-C3E-C2E
4	A	903	LIL	C3E-O2E-C1F-O1F

There are no ring outliers.

4 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	750	FCI	2	0
4	A	903	LIL	11	0
4	A	904	LIL	10	0
6	A	906	LIM	6	0

5.7 Other polymers (i)

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	695/705 (98%)	-0.19	7 (1%)	84	85	31, 62, 94, 113	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	412	HIS	6.7
1	A	566	PHE	2.9
1	A	493	TYR	2.5
1	A	677	ARG	2.4
1	A	403	TYR	2.3
1	A	78	VAL	2.2
1	A	452	ASP	2.0

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

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

6.3 Carbohydrates

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	KDO	A	1002	15/16	0.97	0.09	-2.15	45,59,70,92	0
2	GP4	A	901	15/16	0.97	0.10	-4.23	32,46,71,73	0
2	GP1	A	902	16/16	0.97	0.08	-	50,63,90,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	GPH	A	1005	17/18	0.85	0.17	-	55,82,120,120	0
2	GAL	A	1007	11/12	0.82	0.28	-	74,96,110,120	0
2	GLC	A	1006	11/12	0.90	0.21	-	74,83,102,110	0
2	GAL	A	1009	11/12	0.84	0.21	-	81,91,107,107	0
2	KDO	A	1003	15/16	0.93	0.13	-	49,64,80,85	0
2	GMH	A	1004	13/14	0.96	0.12	-	43,59,80,83	0

6.4 Ligands

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
4	LIL	A	903	31/32	0.92	0.40	13.72	48,78,93,96	0
6	LIM	A	906	17/18	0.93	0.37	8.43	54,65,82,97	0
4	LIL	A	904	31/32	0.94	0.30	7.64	48,59,76,83	0
8	FCI	A	750	46/51	0.98	0.19	0.13	21,47,64,69	0
3	NI	A	1011	1/1	0.96	0.08	-	98,98,98,98	0
7	EA2	A	1008	11/12	0.93	0.16	-	52,109,120,120	0
5	AAE	A	905	6/7	0.90	0.20	-	75,80,86,107	0
3	NI	A	1012	1/1	0.95	0.10	-	113,113,113,113	0

6.5 Other polymers

There are no such residues in this entry.